

VINE – A NUMERICAL CODE FOR SIMULATING ASTROPHYSICAL SYSTEMS USING PARTICLES II:
IMPLEMENTATION AND PERFORMANCE CHARACTERISTICSANDREW F. NELSON^{1,2}, M. WETZSTEIN^{3,4}, AND T. NAAB^{4,5}*Draft version July 10, 2009*

ABSTRACT

We continue our presentation of VINE. In this paper, we begin with a description of relevant architectural properties of the serial and shared memory parallel computers on which VINE is intended to run, and describe their influences on the design of the code itself. We continue with a detailed description of a number of optimizations made to the layout of the particle data in memory and to our implementation of a binary tree used to access that data for use in gravitational force calculations and searches for SPH neighbor particles. We describe the modifications to the code necessary to obtain forces efficiently from special purpose ‘GRAPE’ hardware, the interfaces required to allow transparent substitution of those forces in the code instead of those obtained from the tree, and the modifications necessary to use both tree and GRAPE together as a fused GRAPE/tree combination. We conclude with an extensive series of performance tests, which demonstrate that the code can be run efficiently and without modification in serial on small workstations or in parallel using the OpenMP compiler directives on large scale, shared memory parallel machines. We analyze the effects of the code optimizations and estimate that they improve its overall performance by more than an order of magnitude over that obtained by many other tree codes. Scaled parallel performance of the gravity and SPH calculations, together the most costly components of most simulations, is nearly linear up to at least 120 processors on moderate sized test problems using the Origin 3000 architecture, and to the maximum machine sizes available to us on several other architectures. At similar accuracy, performance of VINE, used in GRAPE-tree mode, is approximately a factor two slower than that of VINE, used in host-only mode. Further optimizations of the GRAPE/host communications could improve the speed by as much as a factor of three, but have not yet been implemented in VINE. Finally, we find that although parallel performance on small problems may reach a plateau beyond which more processors bring no additional speedup, performance never decreases, a factor important for running large simulations on many processors with individual time steps, where only a small fraction of the total particles require updates at any given moment.

Subject headings: methods: numerical — methods: *N*-body simulations

1. INTRODUCTION

In a companion paper (Wetzstein, Nelson, & Naab 2008, hereafter Vine1), we describe the physics implemented in our numerical code, VINE, the integrators used to evolve systems forward in time, the implementation of hydrodynamics using SPH (Smoothed Particle Hydrodynamics), the gravitational force solver and of the implementation of periodic boundaries. We also describe several test problems on which we demonstrate the code and its performance relative to the Gadget 2 code of Springel (2005). In this paper, we describe our implementation of the techniques used to calculate gravitational forces and determine neighbors needed for SPH calculations. We also discuss in detail the optimizations made to maximize the code’s performance.

In order to maximize scientific productivity, a numerical code must be able to perform simulations with the lowest possible computational expense while still main-

taining an accurate realization of the evolution. The exact definition of an ‘accurate realization of the evolution’ will in general be problem dependent: for one problem, one technique might yield entirely acceptable results, while for another it produces nonsense. VINE has been designed to be both very flexible and very modular, in order to allow the choices of specific algorithms to be made by its users, rather than by its writers. If one algorithm or setting turns out to be inappropriate, another may easily be selected or added to the code.

Of the two main components in the particles’ integration schemes, update and derivative calculation, the latter is by far the most computationally expensive, but the former may have greater influence on the total run time. For example, stability properties may require smaller time steps be made with one integrator rather than another, or one integrator may require more derivative calculations per time step than another. In Vine1, we discussed the two integrators implemented in VINE, each of which require different constraints to obtain a given computational accuracy at a given expense. We also described our implementation of an individual time step scheme, by which each particle can be evolved forward in time at its own rate, greatly reducing the total computational expense when systems with large dynamical ranges are modeled.

In this paper, we focus our attention on techniques

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that can make derivative calculations more efficient. Our purpose will be twofold. First, we describe our implementation of a binary tree based scheme for efficiently determining gravitational forces on particles and lists of neighbors particles for use in SPH calculations and the alternative options we have implemented for using special purpose hardware for those calculations if it is available. Secondly, because efficient calculations require both efficient algorithms and efficient implementation of those algorithms on computational hardware, we describe in some detail the the low level optimizations we have implemented to improve the performance of the code itself on modern, microprocessor based computers. It is our hope that in describing the optimizations in detail, other users of VINE will come to understand the principles important for obtaining good performance, so that they are able to incorporate features of their own into VINE with comparatively little effort, and with equally optimized performance. Alternatively, because we recognize that some may have considerable investments in their own codes, our descriptions may be of use in making incremental modifications to those codes that also improve performance.

We begin in section 2 with a discussion of the properties of the computers on which we expect that VINE will be used. In section 3 we describe the construction of the binary tree used to organize particles so that calculations may be performed efficiently on them. In section 4, we describe efficient methods for accessing the data in the tree, and in section 5 we describe optimizations of the calculations themselves. Next, in section 6 we finish the description of VINE with an overview of the code itself and the hardware requirements needed to run a simulation of a given size. The overall performance of each of the four major portions of the code that interact with the tree is described in section 7, including a discussion of parallel efficiency and tunable parameters to increase performance. Finally, in section 8 we summarize the features of VINE, suggest further improvements that may be made to it and give a web site where the code may be obtained electronically.

2. PRACTICAL ISSUES RELEVANT FOR OBTAINING GOOD PERFORMANCE

Because efficient computation requires knowledge of both the calculations being performed and the machines on which they are performed, we describe here some of the more important properties of the computers on which we expect this code to be run, and the impact that their strengths and limitations have for the design of the code.

We have designed VINE to run efficiently on microprocessors commonly used in workstations and shared memory parallel computers. If available, and at the user's option, VINE can utilize special purpose 'GRAPE' hardware to calculate mutual gravitational forces of particles on each other. In this section, we review some of the most significant architectural features of systems employing such hardware, describing their strengths and limitations. We will conclude by pointing out constraints that motivate some of the optimizations in VINE.

2.1. Running simulations on one processor

Without question, the most important hardware constraint we encounter in optimizing VINE for fast perfor-

mance is that imposed by memory latency. As a class, all microprocessors share the constraint that loading or storing a value to or from memory is much more expensive than, for example, adding them together. Depending on the processor, a single calculation may take one or at most a few clock cycles, and several calculations may be processed at the same time on the same processor. On the other hand, loading and storing may take as many as hundreds or thousands of clock cycles. The universal solution has been to incorporate relatively small caches of memory into the processor itself, from which values can be accessed very quickly, assuming that they are already present in the cache.

Typically, modern processors include two or more levels of cache, labeled 'L1', 'L2' etc, which are divided into a number of 'lines' and 'sets'. The L1 cache is the smallest and fastest and higher cache levels are slower and larger. A cache line consists of $\sim 32 - 128$ bytes of memory and is the smallest increment of information that can be loaded into or stored from that cache at a time. Even if a program requires only a single value from a given range of memory, say a single integer (4 bytes) or a single double precision (8 bytes) real value, that load also brings several additional, possibly unneeded values into the cache. Any given address in main memory can be loaded into any one of exactly n_s lines, where n_s is the number of sets (the set 'associativity'). Typically, $n_s \sim 2 - 4$.

For larger scale memory requirements, processors access a main memory, for which access times are much longer. In practice, access to the entire memory at one time does not occur because a translation must be made between the virtual address by which the program refers to some value and the physical address at which that value is actually stored. The processor holds a finite number of such translations to 'pages' of main memory which, depending on the system, may be as small as 4 kB or as large as 32 MB and on some, may even be selected at run time by the user for a given job. The processor stores the address conversions for a number of virtual/physical pages in a special cache called the 'Translation Lookaside Buffer' (TLB). Accessing a value resident on a page already mapped by the TLB, but not currently resident in cache may take as many as a few hundred clock cycles, due to the slower speed of main memory relative to the processor. Accessing a value from a page not resident in the TLB requires in addition that a new address translation be calculated, replacing replace one of those currently in residence in the TLB. While some processors have special circuitry to assist in the calculation so that it adds only a small additional delay, others require an intervention by the operating system, resulting in additional delays of a few hundred cycles.

2.2. Running simulations with GRAPE hardware

The most costly component of simulating any system including self gravity is the calculation of the mutual gravitational forces of particles on each other. While costly, it is also simple to describe and implement, and therefore lends itself to a specialized solution. Rather than perform the calculations on a general purpose processor used for all the calculations, special-purpose processors called GRAPE (for **GRA**vity **PI**PE) have been developed (see e.g. Sugimoto et al. 1990; Makino & Taiji

1998) to perform the gravity calculation instead.

Although GRAPE hardware is specifically designed to accelerate computation of gravitational interactions, it cannot perform any of the other calculations required for the simulation to proceed. It must therefore be attached to a general purpose computer (the ‘host’) and data must be sent to it for calculation, then results returned to the host for use in the rest of the calculations. In some circumstances, the data transfer time (i.e. the ‘memory bandwidth’) can in fact be comparable to or greater than the calculation time, due both to the actual transfer speed and to latencies required to begin or complete each transfer. An important example of such inefficiency will be when only a few particles require force calculations, such as will occur when individual time steps (see Vine1) are used in a simulation, or when the interaction lists are relatively short, such as will occur when the hardware is used in combination with a tree.

Another limitation of GRAPE systems is that they implement a reduced precision internal numerical representation, which constrains the dynamic range of the input data (particle masses and positions) and increases the errors in forces returned. GRAPE-3 (Okumura et al. 1993) for example, produces errors of order of 2%, while GRAPE-5 (Kawai et al. 2000) produces errors of 0.3%. On the other hand, even numbered revisions, such as GRAPE-2 (Ito et al. 1991), GRAPE-4 (Makino et al. 1997) and GRAPE-6 (Makino et al. 2003), implement much higher internal precision numerical representations, and do not produce such large errors.

Because the errors in the reduced precision variants are uncorrelated, they do not impose problems for the time evolution of collisionless simulations (Makino et al. 1990), and may be used without difficulty in models of such systems. On the other hand, the high precision GRAPE variants may be used to model both collisionless and collisional systems such as stellar clusters, where individual particles in the simulation represent individual stars in the cluster.

So far, a number of simulations using GRAPE processors in combination with the tree and individual time steps have been performed using VINE (Naab & Burkert 2003; Naab et al. 2006a; Bell et al. 2006).

2.3. *Running simulations on many processors in parallel*

Even with the fastest processors available, the time required to perform simulations of systems at high resolution may exceed the time that the scientist running the simulation can remain patient. Fortunately, the required work can be shared among more than one processor so that time required becomes much smaller, and parallel computing architectures are commercially available at costs that make them affordable for use in scientific research.

In the abstract, work required to complete a given task must be divisible into sub-units that are independent of all other such units in order to run correctly in parallel, and those sub-units must be parceled out to be run at the same time on different processors. Data required to complete the task must not be changed while any work remain incomplete and the relevant results of previous tasks must be communicated to different processors, so that a single coherent picture of the entire simulation exists at all times. In order to run efficiently, the work

units must be of similar size, so that they can be divided evenly between all processors and so that little time is wasted while some processors sit idle and others complete disproportionate shares. Secondly, communication must be fast, so that relatively little time is spent synchronizing the results of different processors. Finally, the amount of work that cannot be broken into independent parts must be small.

For shared memory systems, partitioning naturally occurs at a very low level in the code, often at the level of individual loops themselves. An important factor limiting performance in this case is that the work per loop iteration can be extremely small, so that the overhead required to distribute work among processors becomes significant. In other cases, parallelizing loops at higher levels of organizational structure may be possible, but will not have identical quantities of work per iteration, leading to load imbalance unless some intelligence can be applied to parceling out each iteration.

Additionally, in large scale shared memory systems that employ so called Non-Uniform Memory Architectures, or ‘NUMAs’, access times to main memory are not the same for all locations, but instead depend on where a particular value is stored relative to the processor that attempts to load it. For simple parallelized loops, such as those used by the integrator to update particle data at each time step, a significant and otherwise hidden source of load imbalance can originate from this source. The same number of loop iterations, containing identical mathematical operations, may require different amounts of time to complete when run on different processors because data required to complete one processor’s iterations are coincidentally found closer to it than are the data required to complete some other processor’s iterations.

Finally, in recent hardware architectures, two or more processor ‘cores’ are present on the same chip, and some components on that chip (e.g. cache, memory controllers, or simply the pins by which data are transferred on and off the chip itself) are effectively shared between several logical processors. If the execution profile of code running on all cores of a chip leads to competition for access to a given resource, then the contention that results will degrade the overall performance of the code. In this context, limits on the overall memory bandwidth of data transferred to the processor may become of particular concern, in addition to the memory latency issues discussed above. Processors may ‘starve’ for work, while waiting for data to be loaded from memory. To date, we have not observed any impacts on the performance in VINE due to such issues however.

2.4. *Implications for designing efficient numerical software*

VINE has been developed for use on single and multi-processor shared memory architectures using the OpenMP (Deagum & Menon 1999) suite of compiler directives to share work among the processors. In this section, we will therefore focus on issues relevant for obtaining good serial and parallel performance on shared memory architectures. We note, however, that many of the issues presented here are common to both shared and distributed memory paradigms, and so many recommendations about optimization strategies will apply to

distributed memory parallelism as well.

Both on small scales and large, memory access latencies dominate the list of performance constraints for large simulations. The two important points to note are that first, accessing cached data is very fast compared to accessing main memory and second, that the caches are typically much smaller than the total memory required for a typical simulation. This means that less immediately needed quantities may be overwritten by loads of other quantities if other calculations require them. Information may need to be loaded into cache from main memory many times if it is required for many calculations. We are therefore well advised to reuse previously cached data to the fullest extent possible before discarding it for other more immediately useful data.

For example, we will often require a calculation of the distance between two particles. In three dimensions, such a calculation requires that six quantities be loaded into the processor for calculation, consisting of the three spatial coordinates of each particle. We might consider storing each component of position in separate arrays, one for each direction. However, this will inevitably lead in practice to six costly loads from main memory for a single distance calculation. On the other hand, with the discussion in section 2.1 in mind, we know that a single load operation will load at least four double precision values from main memory into the L1 cache. If we instead store particle positions in adjacent memory locations, then all three coordinates can be loaded into the L1 cache with a single load from main memory, and the second and third loads to the processor are nearly cost free because they are already resident in L1. In this context, a two dimensional array with one dimension corresponding to the x , y or z component of the position, and the other to the specific particle, fits our requirements exactly if we also take care to arrange that the ‘fast’ index (which, because VINE is written in Fortran, will be the first) defines the position components, and the slow index defines the particle.

On a more general level, we will frequently require that the same values be accessed many times. For example, spatially adjacent particles will have nearly identical lists of neighbors for SPH calculations and nearly node interaction lists for gravity calculations. All calculations involving those lists must load the same quantities for these particles many times. As Warren & Salmon (1995) point out, if we can arrange that their data can remain in cache after their first load from main memory, the calculations will proceed much faster. Two optimizations are possible here, implemented not only here, but in other codes as well (Warren & Salmon 1995; Springel 2005; Stadel 2001). First, we note that if we can arrange that neighbor searches for one particle, be immediately followed by neighbor searches for a nearby particle so that the data for their nearly identical neighbor lists (and prospective neighbors) are already in cache, then calculations using those data will proceed much faster due to decreased load times. Second, if physically nearby particles are also located nearby in the system’s memory, then the correlated spatial positions and memory locations ensure that data are ordinarily found on the same set of physical pages in memory, providing better cache reuse and fewer TLB misses. In section 3.5, we describe how sorting the particles and tree nodes accomplishes both optimizations.

On still larger scales, tree traversals will span huge ranges of physical memory, but access data in that memory only sparsely and perform only a small number of calculations per access. The actual calculation of gravitational forces will span similarly large ranges of memory, with only slightly more calculations per access. For example, a typical calculation of the gravitational force on a particle in a simulation comparable to one of our test simulations in section 7.1 below, will require the summation of multipole moment contributions from several hundred to several thousand nodes and atoms, and require several times this many nodes be examined for acceptability. Although the quantity of data for these nodes is comparatively small, it is spread thinly over a volume of memory that may be many gigabytes in size. As a consequence, consecutive calculations will lose all benefits from cache or TLB reuse even if done for particles with identical interaction lists. The size of an interaction list means that interaction data near the beginning of a list will be evicted from cache by data near the end of the list, requiring that it be reloaded when the second particle’s force is calculated. The same effect will occur in the TLB, with address translations for later nodes in the list evicting those that came earlier.

Two straightforward optimizations to the code itself and a third hardware optimization both increase the raw speed of the calculations and reduce the impact of sparse memory access patterns substantially. First, sections 4.2 and 4.3 describe a method for performing a single tree traversal for groups of particles at the same time, reducing the overall number of redundant accesses to tree data. Second, section 5.1 describes a method for loading small segments of the full interaction list data into a small temporary array tuned to the size of the L1 cache, which is then used for calculations on many particles occur before being discarded in favor of later nodes in the interaction list. Finally, we utilize the option of using large hardware pages on systems where they are available and can be used efficiently.

Sections 7.3.2, 7.3.3 and 7.3.4 describe the benefits realized by each of the optimizations discussed in this section on the gravity, SPH and tree build calculations which are, respectively, the three most costly operations in particle simulations. Each of the memory management optimizations discussed above will also act to avoid memory latencies inherent in NUMA systems as well, by concentrating memory accesses in a small, moving footprint that is accessed repeatedly. Therefore, optimizing the code for high performance in serial mode will have the additional benefit that parallel performance may also benefit.

3. BUILDING A TREE: ORGANIZING PARTICLES FOR EFFICIENT ACCESS

As we discussed in Vine1, lists of neighbor particles and approximate gravitational force computations can be obtained with the help of a tree data structure to organize particles. Using a tree, groups of particles that may potentially interact with another may be qualified or disqualified with a single calculation, using a node in the tree as an approximate substitute for some large number of exact interactions.

A variety of techniques for building and implementing tree structures have been discussed in the literature.

One common technique (Barnes & Hut 1986) (hereafter a ‘BH tree’) builds the tree in a ‘top down’ fashion by artificially tessellating space into successively smaller cubes. The first cube contains the entire system of particles and if any cube contains more than one particle, it is split into eight smaller cubes of equal volume (hence the name oct-tree for this type of tree structure). The procedure is repeated until the cubes on the lowest level (the leaves of the tree) contain either exactly one particle or no particle at all. A similar technique originating in Bentley (1979) is used in the PKDgrav code (Stadel 2001) and its later incarnation, Gasoline (Wadsley et al. 2004), which also includes hydrodynamics with SPH. This tree algorithm builds a balanced, so called ‘ $k-d$ ’ tree (referring to k data per node in d dimensions), by recursively bisecting space. The tree is constructed from top down, by choosing a direction (typically the direction for which particles are most extended in space) along which to bisect the population of particles, so that half of the particles lie on one branch of the tree and half on the other. A third technique (Press 1986; Jernigan & Porter 1989; Benz et al. 1990), occasionally referred to as a ‘Press tree’ in honor of one of its inventors, builds a tree from the ‘bottom up’ by associating mutual nearest neighbor particles or nodes with each other as successively higher nodes in the tree until only one node is left. Since exactly two particles or nodes are grouped together, the latter two types of trees are commonly grouped together and called binary trees.

In this section, we first briefly discuss some literature debating the merits of each of the above tree algorithms and some reasons for choosing the Press tree for use in VINE, followed by a description of the method used to construct the tree used in VINE. Because the details of the tree structure itself will have a major effect on the total run time of the rest of the code, we will outline our tree construction and post processing in some detail, although many aspects of it may be found in the references above.

3.1. What kind of tree is best?

Use of tree based force calculation algorithms for N -body simulations became common beginning in the 1980s (see citations above), and debates over which sort of tree algorithm is better or worse for which sort of calculation have continued since that time. We attempt here to summarize some of this debate and the choices that influenced our decision to continue using the Press tree, present in versions of the code on which VINE is based (Benz et al. 1990).

The basic metric for the quality of a given tree algorithm can be summarized essentially as a statement of the science goals of the tree code’s user: more, and more realistic, simulations of interesting physical systems are better. Therefore, when used as a tool to accelerate calculations of interparticle forces, the best tree algorithm is the one which produces more accurate (or at least ‘accurate enough’ for a given problem) forces more quickly than any other, so that more and larger simulations can be completed in a given time. Unfortunately, this metric has not always been used in studies of tree code quality, sometimes leading to conclusions that directly contradict each other.

For example, a study by Anderson (1999) compares the

performance of BH trees with $k-d$ trees using largely analytic arguments. He concludes that a spatially balanced⁶ $k-d$ tree will provide performance superior to that of a BH tree. In contrast, Waltz et al. (2002) compare a BH tree to a $k-d$ tree in direct code to code tests but make the opposite conclusion, that BH trees ordinarily provide superior performance to $k-d$ trees.

We can begin to resolve the contradictions by examining the metrics used to define better performance in each case. For example, Anderson (1999) uses the average length of an interaction list as a proxy metric for the actual calculation rates, neglecting the cost of tree traversals entirely. He finds that $k-d$ tree traversals result in shorter lists, meaning that $k-d$ trees are preferable. On the other hand, Waltz et al. (2002) use the average number of nodes touched during a traversal as their primary metric. They find that several times more nodes are opened in binary trees than in oct-trees, meaning that oct-trees are preferable. In fact, in terms of the interaction list lengths, the results of the two studies actually confirm each other—Waltz et al. (2002) also find that lists some 20-30% shorter result from $k-d$ trees, but attach little weight to this fact in their conclusions.

Interpreting these conclusions in any general case depends strongly on how well the proxy metrics actually correlate with the total cost of a calculation. In other words: are the metrics relevant only for a given study, using a given code? Given the conclusions, we may reasonably infer that Waltz et al. (2002) found that traversals were the dominant calculation cost, while Anderson (1999) found the opposite, which lead directly to their opposing conclusions. However, neither the Anderson (1999) nor the Waltz et al. (2002) studies discuss the relative costs of traversal and evaluation in any detail and further, it is not clear that their results are generalizable. For example, few codes in common use implement the comparatively costly ‘priority queue’ node opening strategy of Salmon & Warren (1994), as Waltz et al. (2002) do. Also, Waltz et al. (2002) make their comparisons to density balanced $k-d$ trees, while Anderson (1999) points out that using this variant may lead both to poor error properties and to lower calculation rates.

A much earlier study by Makino (1990a) appears to be more generally applicable, and compares the performance of a BH tree to a Press tree. His results are largely consistent with the later studies in that he too finds many more nodes need to be opened for the case of the binary tree, but that shorter interaction lists are required to provide the same force accuracy. As a result, the per interaction cost is some 50% larger for the binary tree than for the Press tree, but since fewer interactions are required, he finds near parity in performance at the same accuracy. He concludes that secondary factors, such as the tree construction cost, become important in decisions to use one or another. Here again, although he notes that Press trees are an order of magnitude more costly to construct, they can be reused while an oct-tree must be rebuilt at each step, so that the cost is amortized. Makino concludes that because the costs of the traversals

⁶ In Anderson’s nomenclature, density balancing is defined by the criterion described in the last section, that nodes at each level contain equal numbers of particles. In contrast, nodes in a spatially balanced $k-d$ tree may have unequal particle counts, and instead divide space equally at each level, as is done in oct-trees.

and force calculations using either method are comparable, and that lesser factors such as the tree construction time are also comparable, the algorithmic efficiency on different architectures may be important in influencing the decision to use one or the other.

We have chosen to implement a nearest neighbor binary tree based on the algorithm described in Press (1986) and Benz et al. (1990) in VINE. Since a consistent conclusion of the studies above is that traversal costs are higher in such trees, we also implement the grouped tree traversal strategy of Barnes (1990), which acts to reduce the costs to more acceptable levels. At settings typical for production use, we will find that those costs are indeed low, at some 10-20% of the total. A nearest neighbor tree also has the advantage that particles tend to be grouped in the tree in the same manner that they are grouped in space, rather than being grouped into artificially bounded cubes in which particles may be well separated in space but still found in the same cube, or quite close but found in different cubes. As an example, consider a centrally condensed, spherical particle distribution contained at the center of a ‘master’ cube. At the very first subdivision of that cube into sub-cubes, particles near the center may be separated into different tree branches, while the nearest neighbor tree instead groups them together. It is therefore a first step towards our goal of performing neighbor searches for adjacent particles at similar times during the full calculation in order to gain the advantages of cache reuse.

3.2. Tree construction

Nearest neighbor tree construction depends upon the ability to efficiently determine the nearest neighbors of all particles or nodes for which no nearest neighbor has yet been found and to associate such pairs into higher order nodes. Both because the exposition in Benz et al. (1990) was quite brief and to describe our modifications to it, we will describe the process we use in detail here.

First, we note that in order to ensure modularity and maximize the efficiency of accessing the tree data, we implement completely independent data structures for the tree and for the driver of the integration. The first action of the tree build routine is therefore to receive a list of positions, masses and smoothing lengths (set to a fixed value for N -body particles) from the driver and store them in dedicated memory local to the tree module, after which the actual construction begins.

Benz et al. (1990) employ a temporary hash grid overlaid on the particle positions to associate each particle with a specific grid zone. Then for each zone, they define a linked list of particles occupying that zone to determine suitably small lists of candidate particles to examine for nearest neighbor status. In spirit, this method is the same as the so called ‘friends of friends’ method (Hockney & Eastwood 1981), but employs a slightly more sophisticated method for defining the hash grid.

We create the hash grid by first sorting the particles’ positions in each spatial dimension, d , and then dividing the sorted lists into $(N_p/n_h)^{1/d}$ equal length sections. The average of the coordinates of the two particles on either side an adjoining section then defines the position of the boundary for each zone in each direction. Thus, the grid is unequally spaced in the positions of each grid

boundary, but equally spaced in number of particles per grid coordinate. The quantity n_h defines the expected average number of particles per zone. Typically we find that an average of $n_h \sim 3 - 5$ is most computationally efficient, but the best hashing factor also depends on the level of particle clustering found in a given simulation.

After creating the grid, we assign a one dimensional coordinate key to each particle, which defines its position in the grid as

$$K_p = i + (j - 1)n_x + (k - 1)n_x n_y \quad (1)$$

where i, j and k are the ordered triple defining a particle’s position, and n_x and n_y are the number of hash grid zones in the x and y coordinate dimensions of the grid. When 2D simulations are performed, $k = 1$ so that the last term is always zero. With a key in hand for each particle, a single loop through the particle list is sufficient to define a set of linked lists containing the particles resident in each hash grid zone. Lists for each zone are characterized by a ‘head-of-list’ node and a zero terminated list of ‘next’ pointers, defining the next node or particle in the list. Traversing the list for a given grid zone is then equivalent to accessing a list of candidate particles within a small, well defined region, as we require. The appropriate list for any given particle is available directly from examining its coordinate key, which identifies the appropriate head of list node.

In order to determine nearest neighbor status from the lists of candidates, we first determine distances to all candidates in a particle’s own zone and the distance to the nearest zone boundary. If any boundary is closer than the nearest neighbor particle so far discovered, then the search region is expanded in the direction of the nearest zone boundary. The search continues until the nearest neighbor is closer than any zone boundary. Once found, we store the nearest neighbor’s identity and continue until we have determined the nearest neighbors of all unassociated particles and nodes.

After all of the nearest neighbors have been found, we check each node for *mutual* nearest neighbor status, defined by the condition that a node’s nearest neighbor has that node as its own nearest neighbor. If the condition fails, the node remains on the unassociated node list until the next round. If it succeeds, we create a new unassociated parent node from the pair and remove them from the list of unassociated nodes. The sibling pointer for each of its two children are updated to point to each other, and a daughter pointer is defined to point to one of the children, defining the ‘left’ child. Each pointer is an integer array whose value contains the array index of the daughter or sibling node (daughter pointers for particles are set to zero). We calculate the mass of the new node and its position is defined as the center of mass of the two children.

The entire procedure is repeated with the remaining unassociated nodes until only one (the ‘root’ node) is left. When complete, the tree consists of exactly $2N_p - 1$ nodes, of which N_p correspond to the original particles (‘atoms’).

3.3. Optimizations of the tree build

So far the tree construction algorithm is identical to that outlined in Benz et al. (1990). Here, we introduce several optimizations of the original method, which

greatly accelerate the construction over that required in the original method.

Using the recipe above, unassociated nodes are examined and nearest neighbors found in an arbitrary order, depending on their location in the list given to the build. Instead, we recognize that the candidate nearest neighbor examinations will be most efficient if nodes that are spatially adjacent are examined consecutively, so that their data are already located in the cache. Therefore, rather than looping over the list of nodes, we loop over blocked sub-regions of our hash grid, examining all nodes in each region before going on to the next. This ordering ensures a high probability that recently examined nodes will still be found in the cache when they are re-examined as a prospective nearest neighbor for a nearby node. In addition, newly created nodes will be placed in nearby memory locations, increasing the benefits of the correlations between memory and spatial locations as the build proceeds to later iterations.

At each iteration of the tree construction, a new grid is created, requiring that the positions of the unassociated nodes be sorted in each direction. Instead of performing sorts at each level, we have found that inserting the new nodes into the original hash grid is a vastly less expensive alternative because the position of the new node is already known and its grid zone can be immediately determined. To retain efficiency as the number of nodes per zone decreases, we revise the hash grid and the associated particle keys by cyclically decreasing the number of zones in each of the coordinate directions by a factor of two.

After the first iteration, the linked lists of unassociated nodes for each grid zone will contain both newly created nodes and nodes for which no associate could be found in the previous iteration. In addition to the head of list pointer for each zone, we also define a head of list pointer for the old nodes on the list, so that we can either traverse the full list of new and old nodes for the zone, or only the new nodes. Distinguishing between old and newly created nodes is useful because no ‘old’ node will be closer to a given node than the nearest neighbor that has already been determined for it. We can therefore reduce succeeding searches for nearest neighbors to the list of newly created nodes as long as the previously identified nearest neighbor also remains unassociated. This optimization is especially beneficial and when the particle distribution is very inhomogeneous, because in such cases relatively fewer new nodes are created per level and many redundant examinations can be avoided.

3.4. Parallelizing the tree build

Building the tree in parallel requires that the work on each level of the construction be divided into three distinct steps, each of which must be completed before the next can begin. First, a nearest neighbor must be assigned for each unassociated node and, second, mutual nearest neighbor status must be determined for pairs of unassociated nodes and a new node created from each pair and, third, newly created nodes must be placed in the hash grid.

Distributing iterations of the loop over sub-regions among processors is sufficient to parallelize the work required in both of the first two steps. A synchronization point is required between the two steps however to en-

sure that all nearest neighbors determinations have been made before any mutual nearest neighbor determinations are made. The distinction is necessary to eliminate a potential race condition that would otherwise exist in the association. Without the synchronization, two nodes residing in different sub-regions (and handled by different processors) that are in fact mutual nearest neighbors could be passed over because one of those nodes has simply not yet been assigned any nearest neighbor at all.

As nodes are associated and created, they must be placed in a specific memory location. An additional synchronization is required in the form of an atomic update to a counter that defines the location of the last node already stored in memory. Each processor increments the counter only one time per level by an amount equal to the number of nodes found in its part of the search. Contention for access to the counter is therefore minimal.

The computational cost of setting up the initial hash grid is dominated almost entirely by the cost of sorting the particle positions in each coordinate direction. We have implemented the parallel quick sort described by Sanders & Hansch (1997), in which particle positions are divided into N_{proc} segments, each of which is sorted on one processor, then merged with a series of $\log_4(N_{proc})$ merge cycles to obtain the final, globally sorted list. Actual placement of particles in the hash grid has not been parallelized because in the current version of the code, we found performance loss rather than gain. Revising the hash grid is parallelized by partitioning the zones along one coordinate dimension among the processors, then re-associating nodes in deleted zones with the newly revised grid.

3.5. Tree post processing: laying the groundwork for efficient access

After the build is complete, we perform a number of post processing operations on the resulting tree in order to prepare it for efficient access and use. In considering what post processing will be useful, we recall our requirement that tree traversals for spatially nearby particles should occur consecutively. A list of nodes and particles sorted according to the order they are encountered in the tree traversal will satisfy this requirement but presumes a tree traversal strategy, which we will discuss in detail in section 4 below. For current purposes, it is sufficient to note that our traversal effectively converts the tree structure into an ordered list of nodes and particles.

Minimally, this conversion requires that the daughter and sibling pointers for each node be re-associated into linked lists, which then define the order nodes are encountered in a traversal. In practice, only the right daughter nodes require re-association if we generalize the definition of ‘sibling’ for right daughter nodes to point instead to its parent’s, grandparent’s (or great-grandparent’s etc) sibling. For consistency, we define a fictitious sibling of the root node, which also serves as the sibling of all nodes on the extreme right branch of the tree.

We extend the conversion process further by actually reordering the placement of the data in the computer’s memory as well, to correspond to the order that data are encountered in a traversal. Then the data for particles or nodes that are nearby in physical space are stored in locations that are nearby in the computer’s memory and

repeated accesses become more efficient. Because the particle data are copied into completely distinct memory locations for use in the tree, there are actually two distinct sets of data that can be reordered independently of each other. First, the data defining the node information in the tree may be reordered, so that calculations accessing the tree are accelerated. Second, the data defining the particles themselves may be reordered, so that calculations that also (or only) access the particle data may be accelerated.

Reordering the tree data requires that we perform a tree traversal (section 4.1 below) that opens all nodes in succession to establish what the optimal ordering will actually be, and that we then relocate each node in turn to correspond to that ordering. During the traversal, we create a list of nodes linking the consecutive ordering of the tree traversal with the arbitrary ordering of the tree as it was built. Each entry in the list then corresponds to a specific tree node and is thereafter identified as such. Pointers to daughter and sibling nodes are similarly identified and the associations of the original ordering are updated to reflect the re-identification.

In practice, we find that both associating the original ordering to the revised ordering is needed, and vice versa, so we create two reordering lists corresponding to each case. We save these lists so that when node data are revised (section 3.7), they can be used to distribute the particle data into optimal ordering for rapid traversals, at the cost of a single copy of the particle data into the tree data structures. Apart from the copy-in process during the tree revision (which must be performed whether or not the tree data are reordered), no references to the auxiliary list are required and there is no cost to the reordering.

Reordering the particle data also requires one full traversal, in order to obtain a list of all particles only, ordered by their appearance in the tree. Once obtained, the reordering requires only a scratch array into which to copy the particle data, then to restore it in the new ordering using the list. Sections 7.3.3 and 7.3.4 describe the benefits of reordering the particle data. The frequency of reordering required to retain these speedups will of course be very problem dependent, however we have found for some typical problems that a frequency of once every few tens to hundreds of time steps is sufficient, so the cost of this reordering is insignificant.

Finally, we create an ordered list of ‘clump’ nodes, which are defined by the condition that each clump node contains N_{c1} or fewer particles, but whose parent contains more than N_{c1} particles or is spatially separated from its sibling by more than a critical distance (specified at runtime). These clumps are used in the tree traversals for the gravity and neighbor search calculations as described in sections 4.2 and 4.3 below. Various traversals used by the code require that clumps be detected during the traversal so that they may be set aside for special handling. In order to allow detection both simply and inexpensively, we further redefine the daughter and sibling pointers to clump nodes to be negative valued integers. Their absolute values are then the true array index of the clump node. Comparison of the pointer to its absolute value then determines a node’s status as a clump or ordinary node.

Taken together, all of the post processing steps de-

scribed in this section require less than 5% of the total time required for the tree construction itself, and so are a small computational expense. We shall show that even this small cost pays enormous dividends when the tree is accessed, making the added coding complexity also worthwhile.

3.6. Data contained in the tree and required by calculations

After construction, a number of other data remain to be calculated for each tree node, including multipole moments and convergence radii needed to determine their acceptability for use in various calculations. We use the composition formulae originally defined in Benz et al. (1990) to determine the mass, position and quadrupole moments of each node, starting from the particle data only. For a node, n , with daughters d1 and d2, these formulae are respectively:

$$M_n = M_{d1} + M_{d2}, \quad (2)$$

$$\mathbf{X}_n = \frac{M_{d1}\mathbf{X}_{d1} + M_{d2}\mathbf{X}_{d2}}{M_{d1} + M_{d2}} \quad (3)$$

and

$$\mathbf{Q}_n = \mathbf{Q}_{d1} + \mathbf{Q}_{d2} + \frac{M_{d1}M_{d2}}{M_{d1} + M_{d2}} \times (\mathbf{X}_{d1} - \mathbf{X}_{d2}) \otimes (\mathbf{X}_{d1} - \mathbf{X}_{d2}). \quad (4)$$

In addition, we require both the actual size of each node and its multipole convergence radius. The size of a node is conservatively specified by the condition

$$h_n = \max\left(\frac{M_{d1}}{M_n}|\mathbf{X}_{d2} - \mathbf{X}_{d1}| + h_{d2}, \frac{M_{d2}}{M_n}|\mathbf{X}_{d2} - \mathbf{X}_{d1}| + h_{d1}\right). \quad (5)$$

The size of individual particles is defined to be either their smoothing length or the gravitational softening parameter ϵ , in the case of N -body particles. Except for individual particles, the node sizes computed using equation 5 is always larger than strictly necessary, but we have found that the computational cost of this conservative definition is not particularly large. An important exception is that we have found it advantageous to specify the node size exactly for clumps and all of their descendant nodes for use in the SPH neighbor searches, because many fewer nodes must be opened and examined. Therefore, for this subset of nodes, we recalculate the size of node, n , as the maximum distance of any particle, i , contained in the node, from its center of mass:

$$h_n = \max_i(|\mathbf{X}_n - \mathbf{X}_i| + h_i). \quad (6)$$

As described in Vine1 (section 4.2), VINE implements three runtime selectable options, referred to as ‘Multipole Acceptance Criteria’ or MACs, for determining the acceptability of a given node for use in the gravitational force calculation on a particle. We refer to them as the ‘geometric’, the ‘SW absolute error’ and the ‘Gadget’ MACs, respectively. Each is based on a different implementation of the convergence radius of a multipole expansion of the force from that node. One datum for each node is required to implement each of the three criteria and, depending on which criterion was chosen by the

user at runtime, VINE selects which of the three data to calculate and store. In each case, only the portion of the criterion that remains invariant for all node examinations is stored rather than the full MAC definition, in order to minimize computational cost during tree traversals. A user defined accuracy parameter, θ , is also required to complete the specification of the criterion, but takes on different interpretations for each of the different MACs, as defined below.

When the geometric MAC is selected, VINE stores the quantity

$$R_{crit} = \frac{h_j}{\theta} \quad (7)$$

for each node j , where θ is interpreted as a user chosen, dimensionless value between zero and one, parameterizing the minimum acceptable distance at which a node may be used in the gravity calculation. When the absolute error criterion of Salmon & Warren (1994) (the ‘SW’ MAC) is selected, VINE stores the quantity:

$$R_{crit} = \sqrt{\frac{h_j^2}{4} + \sqrt{\frac{3\text{Tr } \mathbf{Q}_j}{\theta}}} \quad (8)$$

where in this case θ is a value defining the maximum absolute error in the acceleration that a single node may contribute to the sum and \mathbf{Q}_j is the quadrupole moment tensor for node j . Finally, when the Gadget MAC of Springel et al. (2001) is selected, VINE stores the quantity:

$$\Phi_{crit} = \frac{M_j h_j^4}{\theta}, \quad (9)$$

where the gravitational constant is set to $G = 1$ and we have replaced the variable R_{crit} with Φ_{crit} in this definition to make clear the fact that the saved portion of the criterion does not have units of length. For the Gadget MAC, θ is interpreted as the maximum magnitude of the relative error in the force allowable to any single acceptable node.

To these, we add an additional criterion that we will find useful, describing the condition that two nodes are in physical contact, or in other words, are ‘neighbors’:

$$r_{ij}^2 < (h_i + h_j)^2, \quad (10)$$

where the nodes’ physical extents are given by h_i and h_j , through either equation 5 or 6. Thus, whether a node actually represents only one or very many particles, the condition for tree nodes to be neighbors is equivalent to the SPH condition that defines neighbor status for individual particles (see Vine1, section 3.2).

3.7. Updating vs. rebuilding the tree

Even though the tree is a nearest neighbor tree, none of the calculations using it require that the nearest neighbor property be satisfied. Therefore we may reuse it in future time steps as long as it remains efficient to do so, revising only the quantities defined in section 3.6 and amortizing the cost of its construction over many time steps. Section 7.3.5 illustrates the conditions that affect the frequency of rebuilds, relative to revisions.

As for the build, when data in the tree are updated, particle data are received from the calling routine and stored (in the sorted tree ordering) in dedicated, locally

defined arrays. Node data are created from the node composition formulae above, with quadrupole moments for particles set to zero. Given these formulae, a necessary condition for creating or updating information for a given node is that all its descendant nodes have been already been updated, and leads naturally from the bottom to top (leaf nodes to root node) update suggested by Hernquist (1990b). We have not found this method to be efficient however, either for updates on a single processor or in parallel, because the work per level is small and the data are widely scattered in memory.

Instead we take notice of the fact that the node re-ordering done to improve performance of the tree traversals can also be used for the tree updates, when used in reverse. In other words, while a tree traversal that starts from the root and opens every node in turn is guaranteed to examine every parent node before its children, a tree traversal that starts from the tree’s termination node and proceeds towards the root is guaranteed to examine every child node before its parent. Structured in this way, a tree update requires a single, long loop over all nodes. Updates for spatially nearby nodes are performed naturally at the same time, allowing substantial speedup due to improved cache reuse. Updates in parallel are done by splitting the tree into approximately equal sized branches, to be handled separately by different processors. A small number of isolated nodes (typically ~ 10) near the root of the tree which cannot easily be associated with any sub branch, are updated in a second, post processing step.

4. TRAVERSING THE TREE

The ultimate goal of any simulation is to model a physical system, so all calculations not leading directly to that end are in some sense wasted. In this context, and even though use of a tree will be enormously beneficial compared to its alternatives, both the processes of building a tree and extracting data from it are wasted: neither is directly related to evolving any particles forward in time or to calculating derivatives for any quantity or particle. Therefore we are well advised to reduce, as far as possible, the time spent in such activities.

Given a tree structure, what is the most efficient way to determine which nodes in the tree are useful as is and which must be refined further? A variety of tree traversal strategies have been discussed in the literature (Barnes 1990; Makino 1990b; Hernquist 1990b; Benz et al. 1990; Warren & Salmon 1995; Dubinski 1996) which are efficient for use on various kinds of hardware, from vector based machines to single CPU microprocessor based machines, to shared or distributed memory parallel architectures. VINE employs elements from several of these methods to obtain various information from the tree. In this section, we first examine a flexible prototype traversal and then describe adaptations of it, used to obtain a variety of information from the tree required for the gravity calculation and the neighbor determination for SPH.

Throughout this discussion, we will refer to a ‘sink’ particle or node to be a point for which data are required from the tree or interaction is to be calculated. A ‘source’ particle or node is an entry in the tree that is tested for or used to determine a contribution to that interaction. In principle, the tree could be traversed and interactions

calculated for any point in space, whether or not that point is actually a node in the tree, however we have implemented only traversals for nodes and particles that are tree members.

4.1. A prototype tree traversal

Traversing a tree requires first, one or more tests that determine the acceptability of a node, second, a prescription for determining which node will be the next to be examined and, finally, a termination condition for the traversal. Without reference to gathering any particular information from the tree, the results of a node examination fall into three categories. A node may either pass or fail its acceptability criterion, or we may defer examination until later based on some other, special property of the node. VINE tests a tree node first for its special properties, then for its acceptability, using the stackless ‘follow the left wall’ rule discussed in Makino (1990b), known more generally as a ‘depth first’ tree traversal. Because it effectively turns the tree traversal which opens all nodes into a space filling curve, in practical effect, this traversal amounts to a variant of the Peano-Hilbert or Morton ordering employed by grid based tree codes (Springel et al. 2001; Warren & Salmon 1995), applicable instead to a nearest neighbor tree.

In a follow the left wall traversal the tree nodes are converted into an ordered list, for which the path of a traversal that opens every node in turn will always take the leftmost branch of the tree that has not already been examined. Accepting a node and advancing to its sibling is therefore equivalent to placing a reference to the node on an interaction list, then dropping some number (> 1) of entries down the list, or exactly one if the node is an atom. The implementation in VINE defines two linked lists which contain respectively, the sibling of the node and its left daughter. We generalize the definition of ‘sibling’ for right daughters to include the parent’s or grandparent’s (or great-grandparent’s etc) sibling, and we use a fictitious node as the root node’s sibling. By extension, the fictitious root sibling is therefore also the sibling of all nodes on the extreme right branch of the tree. Fortran pseudo-code illustrating a traversal using each of the three alternatives is shown here:

```
do while( not finished )

  if( defer? )then

    YES: store node on special treatment
    list and advance to sibling

  elseif( accept? )then

    YES: store node on interaction list
    and advance to sibling

  else

    NO: advance to left child

  endif

enddo
```

Figure 1 shows an example traversal through the tree

structure under the assumption that the ‘special’ characteristic of a node is that it is a particle and the termination condition that the next node to be tested is the fictitious node, so that we traverse the entire tree. For the purposes of this illustration, we do not need to specify the acceptance criterion. Although any property of a node may be used to determine its special character, we choose the fact that it is a particle for simplicity of illustration here. In practical use, this property could be used to differentiate between particles which require treatment as neighbors, and those which do not. A decision about this treatment might be deferred to permit either the traversal code or the neighbor determination to be optimized (or both) by the compiler.

Starting from the root node, we descend one level to its left daughter node. The node does not need to be deferred (i.e. it is not a particle) and we will assume that it is also not acceptable, so control descends again to the left daughter node, labeled ‘A’. Here we will assume that node A is acceptable, and we place it on an interaction list. Rather than descending further (the dashed arrow), control passes instead to its sibling, and upon failing the acceptability criterion descends two levels until we reach node ‘B’, which is a particle and therefore a decision regarding its interaction can be deferred. It is placed on the deferred interaction list, as is its sibling, and control passes onwards to node C, which we will assume is acceptable and place on the normal interaction list. Note here that control would have passed to the same node, labeled D, had any of the previous examinations of C’s parent nodes produced an acceptable result, bypassing all examinations of their daughter nodes. Continuing on, we examine D and upon finding it unacceptable, pass control to its daughter and eventually to node E, which we place on the interaction list. Since the next node examination is the fictitious termination sibling, the traversal is complete.

In principle, one or more tests may be required in any particular traversal to determine the node’s special properties, its acceptability or the ‘not finished’ condition. The flexibility to choose different criteria but keep the same basic traversal strategy allows us to tailor tree traversals individually for different requirements. Two examples of such flexibility are important to point out for VINE users.

First, by changing the starting and termination nodes, we may design a search to traverse all or any part of the tree. For example, in the prototype above, we traversed the entire tree starting from the root using the condition that the last node to be examined is a fictitious termination node. If we had desired instead to search only some portion of the tree, say all of the nodes and atoms beneath node C, then we might choose arrival at node D as our termination node and start the tree traversal at node C. These partial traversals will be important for the close portion of the traversal for gravitational forces and for neighbor searches in SPH calculations. Second, by changing the special property, we can detect atoms very inexpensively (i.e. as nodes with no children), or we can detect ‘clumps’ as defined by the condition that the (integer valued) pointer to the next node and its absolute value are unequal. Later traversals of the deferred nodes may use the same or entirely different criteria from the full traversal used to obtain them originally.

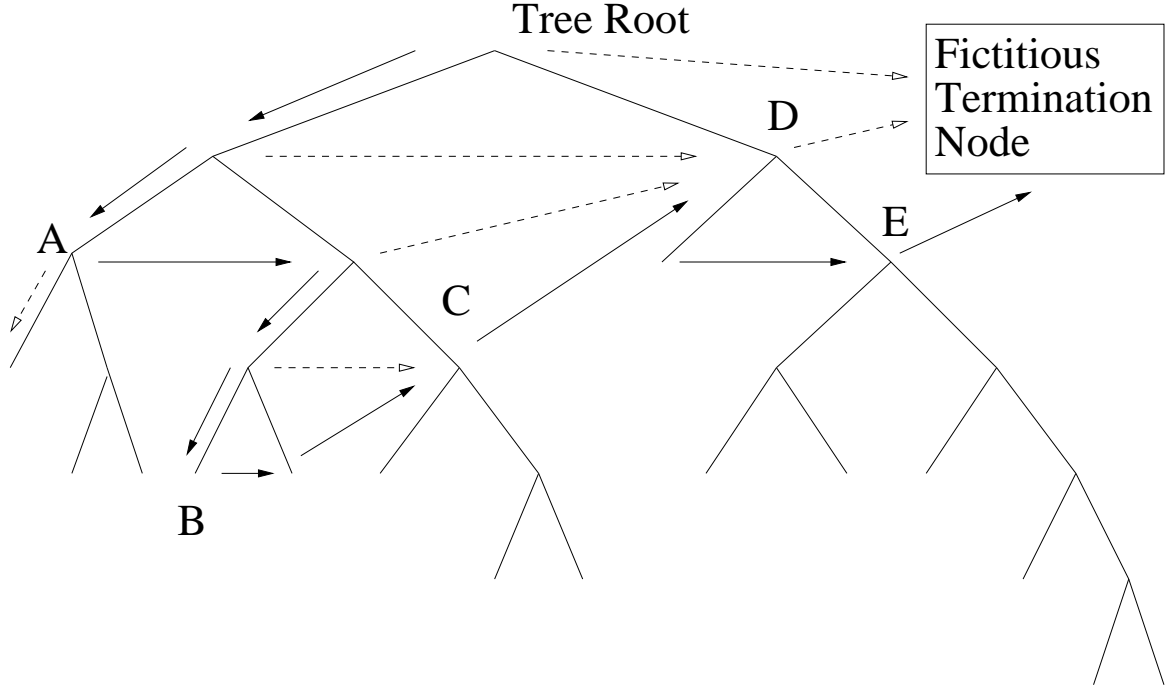


FIG. 1.— Graphic description of the follow the left wall tree traversal used in VINE. The direction taken after each node examination is shown with a solid arrow, while the discarded direction is shown with a dashed arrow.

4.2. Finding acceptable nodes and atoms for the gravity calculation

In order to determine lists of acceptable nodes and atoms for gravity calculations, we must adapt the prototype tree traversal above to the problem at hand and specify acceptance criteria for a node to be used. For the calculation to proceed quickly, we would like to perform as few traversals as possible and accept the minimum number of nodes necessary to produce accurate forces.

We address the first constraint by combining our tree traversal with a variant of the procedure of Barnes (1990), who showed that it was efficient to perform a single tree traversal and obtain a single list of acceptable nodes and atoms for groups of nearby particles at the same time, rather than for individual particles separately. Following this observation, we group nearby particles into ‘clumps’, as defined in section 3.5, and divide each tree traversal into two distinct steps corresponding, respectively, to interactions with distant particles or to close particles.

In the first step, VINE employs a single tree traversal designed to obtain a list of nodes that are certainly acceptable for all particles in the sink clump using the user specified MAC, and a list of neighbor clumps, defined as clumps which pass the criterion in equation 10. In the second, VINE performs individual traversals for each particle in the sink clump, over the list of neighbor clumps. Identical acceptability criteria are used in both steps, but the deferral and termination criteria are specific to each. We find that this division of work allows the total number of traversals to be substantially reduced, so that the fraction of time spent in traversals is only $\sim 10 - 20\%$ of the total required for the entire gravity calculation.

The far traversal uses each clump in the tree in turn as the sink for the gravitational calculation. It extends from the root to the termination node and uses the deferral

criterion that any clump nodes found during the traversal are set aside for later processing during the second step. The node acceptability criterion results in a list of all non-clump nodes encountered that are acceptable for the gravity calculation for all particles in the sink clump. It is impossible for a list of atoms to be generated during this traversal because every particle is a member of a clump and so is set aside, so no other criterion is required to handle them.

The close traversal step divides the sink clump into individual sink particles in turn, and traversals over every neighbor clump complete the interaction lists for each particle. The traversals proceed from each neighbor clump and terminate on its sibling, with the special property set to determine whether the node under examination is actually a particle. They use the same acceptability criterion as the far traversal, with an individual particle now replacing a clump as the sink. Acceptable particles and nodes are placed on a list of atoms or nodes as appropriate.

4.3. Finding neighbor particles for SPH

As for the gravity calculation, VINE’s search for the neighbor particles required for SPH calculations uses a two step far/close traversal strategy. Here again, dividing the traversal into near and far components permits a substantial reduction in the total work required to collect neighbors for the SPH particles. In the far traversal, we obtain a list of all clumps which are neighbors of our sink clump, and in which all possible neighbor particles will be found. Since this traversal is done for an entire clump of particles at a time, its costs per particle are small because they are amortized over the whole clump. Close traversals require searches over only the comparatively small set of neighbor clumps to obtain lists of actual neighbors, for each active particle.

For both near and far traversals, we desire an outcome

exactly opposite to that in the gravity calculation. Instead of storing distant nodes on a list to be processed later, we discard them, keeping only nodes which are close. Because of this difference, we have found that, in the case of far traversals, searches based on the template in section 4.1 are actually less efficient than the level by level (‘breadth first’) strategy of Hernquist (1990b), mainly because the latter permits VINE to retain information from one traversal to the next. We have therefore implemented it as follows.

For a given sink clump, we first create a list of all its ancestor nodes at every level in the tree. Then, for the ancestor on a given level, we test the acceptability of a list of prospective nodes also on that level (i.e. that the node and the sink clump’s ancestor are neighbors according to equation 10. If any node is too distant, we discard it, otherwise we store its children on a stack, or defer further examination if the node is a clump. Once all nodes are tested on a level, we descend to the next, where the process repeats until no nodes remain to be examined. We thus define a progressively more restricted list of acceptable nodes for the ancestors on each level in which all neighbors are to be found. Upon completion, we test all clumps for neighbor status, returning a list to be used in the close traversal step. This strategy permits later far traversals to begin at some lower tree level, defined by an ancestor node shared by the current sink clump and the previously completed sink clump traversal, for which a more restricted set of prospective neighbor nodes has already been determined.

Given a list of neighbor clumps, we proceed to the close traversal phase. For each active particle in the sink clump, each neighbor clump is examined for neighbor particles, using a variant of our prototype. The opening criterion is defined again by status as a neighbor according to equation 10. The deferral criterion by the condition that the node is a particle of the same species as the sink particle, i.e. both source and sink particle must be either both SPH or both N -body particles. When the traversals are complete, we examine all deferred particles for neighbor status at the same time, thereby permitting code optimizations to be made which improve performance.

VINE recalculates neighbor lists each time they are needed even though, in principle, such redundant neighbor recalculation is expensive and therefore to be avoided. On-the-fly recalculation does however provide a substantial benefit to the memory footprint used by the code, because we do not require a large amount of additional memory be allocated to storing lists of every neighbor for every particle. Further, we estimate that 30-40% of each neighbor determination is actually spent calculating quantities required for the SPH calculations anyway. To make most efficient use of these calculations, the neighbor search therefore returns not only the neighbor identities but also the additional information used in the SPH calculation. Specifically VINE returns the mass, squared mutual smoothing length and distance, as well as the components of the distance and the identity of each neighbor particle are stored and returned to the driver SPH routine for use in further calculations.

4.4. *Parallelizing the traversals and their associated calculations*

Both tree traversals and the later calculations using data derived from them are independent of all similar traversals, and produce results that are stored unique locations as well. Moreover, tree traversals are ‘read only’ in the sense that no data contained in the tree are altered. The most natural parallelization strategy will therefore be to define a loop over all clumps in which one traversal and all associated calculations are performed in each iteration. Then the work can be parallelized by distributing different loop iterations to different processors.

We have parallelized both the gravity and SPH density and force calculations in this manner. Each iteration of the loop first calls a routine responsible for the far traversal, then for the close traversal and finally for the actual summation of terms. Lists of acceptable nodes and atoms are stored in data structures private to each processor. Data describing the neighbors for each SPH particle are similarly defined privately for each processor.

In general, the time required to complete an iteration of the loop will neither be fixed nor can it be determined easily from a count of the number of particles in each clump. This is important because load imbalance between different processors will develop if clumps handled by one processor have require a systematically larger amount of work than those handled by another. We might expect that such effects would tend to average out in large simulations and, indeed, to some extent they do if a large enough fraction of particles are active. We use the OpenMP ‘dynamic’ scheduling option, in which loop iterations are parceled out among processors as they become idle, to improve upon this average and retain load balance even when relatively few particles are active.

5. GRAVITY

In this section, we describe the options available in VINE to calculate the gravitational forces, using either information obtained from the tree traversals described in sections 4.2, a direct summation by either the processor or based on special purpose ‘GRAPE’ hardware, or a combination of both.

5.1. *Forces obtained from the tree based calculation*

VINE computes accelerations for all active particles in a clump at one time, using identical interaction lists for the far component of the traversal but distinct close interaction lists. For sufficiently large simulations (\gtrsim a few $\times 10^5$ particles), the interaction lists will typically contain a few hundred to as many as several thousand entries. Although the node data corresponding to these entries may total only a few tens or hundreds of kilobytes (quite small given the memory sizes of today’s computers), it will certainly be much larger than can be accommodated in the fastest level of the computer’s cache hierarchy. More importantly, it will sparsely sample a set of memory locations spread out over many gigabytes of system memory, with only one or at most a few entries resident on any single page. As the summation for each particle proceeds, data for each node must be retrieved either from a page of main memory or from secondary/tertiary caches, stored in primary cache and operated upon by the processor, only to be evicted by later data in the interaction list and retrieved again for the next particle, an effect known to computer scientists as cache or TLB

‘thrashing’. We present in this section two optimizations that substantially mitigate both sorts of thrashing.

First, we note that our tree traversal is split into two steps corresponding to far and near interactions and that it produces identical node lists for the far step. This means that an additional optimization, referred to by computer scientists as cache blocking, can be made that largely eliminates both types of thrashing. Specifically, we allocate a small array whose dimensions have been chosen to be exactly the size of the L1 cache (or more precisely, to the nearest integer multiple of the required single node data volume which is smaller than the L1 cache size) and load a subset of the node data from our list into this array. We then cycle through these data for all of the particles in the clumps that require accelerations. When calculations for all particles have been completed, we discard the subset and reload the array with another subset of the nodes, repeating until the list has been fully exhausted. This strategy avoids TLB and cache thrashing effects during the computations, because the required data will almost always be accessed from an array resident in the fastest level cache available. A small number of cache misses may still occur, because in addition to these node data, the components of position, and the so far accumulated components of acceleration and gravitational potential of the particles for which calculations are being performed will also be accessed frequently in the calculation loop. Typically, however, these data will be accessed so often as to be permanently resident in the registers of the processor, thereby limiting thrashing from this source.

Although we will find that cache blocking is highly effective in the force calculation itself, it can do nothing for the tree traversals, from which the node data are obtained because, by their nature, they sparsely sample very large volumes of memory only once per traversal. Nearly every node examination will then require a new TLB entry to be calculated and one or more new cache lines to be loaded. While few remedies may improve the performance of the cache behavior, the effect of TLB thrashing can be mitigated substantially on hardware architectures for which large pages are available and can be accessed easily by user programs. For a traversal of a tree of a given size, the probability that two or more nodes examined during the traversal will be found on a single page will be higher if the page size itself is larger, so that fewer are required to span the entire data set defining the tree, and fewer TLB recalculations must be made. The magnitude of the mitigation will be dependent on the cost for a TLB recalculation, the simulation size and on the accuracy required for the forces, since higher accuracy will translate directly into more node examinations and longer interaction lists.

5.2. Forces obtained via direct summation

VINE includes a run-time switch to calculate gravitational forces via direct summation, using either the general purpose processor on which all other calculations are made, or GRAPE hardware if it exists.

5.2.1. Using the host processor

VINE includes a run time option to calculate gravitational forces via direct summation, using the general purpose processor on which all other calculations are

made. Although it is indeed simple in practice to compute gravitational forces by direct summation, it is much more difficult to make that computation fast. At its simplest, the summation is characterized by repeatedly cycling through the entire list of particles, incrementing a partial sum of the acceleration on one particle at a time until the list is exhausted, then repeating the process until accelerations on all particles have been calculated. On modern microprocessors, this method suffers from the fact that it makes absolutely no use of the available cache memory to store data that are used more than once.

When accelerations on many particles are required, it is possible to speed up the calculations substantially by using the same cache blocking techniques that were employed to speed up the approximate calculation as described in section 5.1 above. Instead of cycling through the entire list of particles one after the other, we load a small number, n_p , of positions and masses into the cache then calculate partial sums of the accelerations on these particles due to the full list of all N_p other particles in the simulation, one after the other. Loads of data for a new particle on the long list occur rarely compared to loads the cached particles, and so are comparatively cheap compared to the number of computations performed using that data. When the list of N_p particles is exhausted, the accelerations for the first n_p particles are complete. We then load a new set of n_p particle data into the cache and repeat the process until the list of all particles is complete.

5.2.2. Using GRAPE hardware

VINE includes compile time options to calculate gravitational forces using versions 3, 5 and 6 of the GRAPE hardware, through calls to a library of communication and calculation routines distributed with the hardware itself. The simplest approach in using GRAPE boards is to sum the contributions of all particles on each other directly. While it does not change the overall $\mathcal{O}(N^2)$ scaling of the algorithm, it provides a much faster calculation due to the much lower coefficient in front of the $\mathcal{O}(N^2)$ term.

The mechanics of the method used to perform the calculations is quite similar to that used for direct summation on the host. Data for fixed number of particles, in this case totaling a few megabytes in size, are transferred to the GRAPE and used as source particles for the calculation. Small groups of sink particles are then transferred and partial sums of the accelerations are calculated on them using the sink nodes in the GRAPE’s memory, then returned to the host and added to the particle’s accelerations there. When all sink particles have been processed for all source particles, the calculation is complete.

5.3. Forces from the combined tree based and GRAPE based approaches

VINE includes a run time selectable option to use GRAPE hardware to calculate gravitational forces from lists of nodes and atoms obtained from a tree traversal, rather than from a direct summation. This combination was first discussed by Makino (1991) and later Athanassoula et al. (1998) and Kawai et al. (2000) reported its performance on GRAPE-3 and GRAPE-5, respectively. Efficient use of the GRAPE/tree option in

VINE requires that the code and its run time parameters be tuned to somewhat different settings than with the tree/host combination because, with the standard settings, the costs of communication with the GRAPE far outweigh any speedups due to the optimized hardware.

In order to reduce the extreme costs of communication between the GRAPE and host, calculations must be performed for a much larger group of particles than will be optimal in the standard form, so that an interaction list of a given size can be reused many more times before being discarded. Communication costs are high because the number of particles on which forces can be calculated with the same interaction list is limited to the population of a clump, which will be ~ 50 particles (section 7.3.1). Costs would be reduced if the maximum clump population were set to very large values, but at the expense of substantially increasing the time required for SPH calculations. To retain both fast gravity and SPH calculation, we define a set of nodes, which we refer to as ‘bunches’, that play the same role as clumps do in the tree based calculation but contain many more particles.

There are two competing effects that change the effective calculation rate. Reducing the bunch population reduces the length of the interaction list used to calculate forces on its particles. Reducing the size of this list is important because it must be sent to the GRAPE, and shorter lists minimize the per-transfer communication cost. At the same time, smaller bunches mean more transfers, because each tree traversal produces a different interaction list so that total data volume sent actually increases. On the other hand, increasing the bunch population reduces the number of transfers, but increases their size because the interaction lists are longer, again increasing the total data volume that must be sent. Minimizing neither the number of transfers nor their size, independent of the other, will produce optimal performance. The total time for one force computation on all particles is instead a complicated function of the size and number of communications with the GRAPE combined with the number of floating point operations needed and the desired force accuracy. The calculation rate also depends on latency and bandwidth of the connection to GRAPE, but because these are mostly determined by hardware (there is a slight dependence on the chip set on the motherboard of the host computer), they are usually beyond the user’s control.

When GRAPE is used in VINE, the far traversals in the gravity calculation proceed as in section 4.2 with the list of bunches used in place of the list of clumps, creating a single interaction list for the entire bunch. Additionally, rather than proceeding to a set of close traversals over neighboring bunches, the far traversal continues until all nodes and atoms outside the sink bunch are determined. Finally, all particles in the bunch are automatically added to the interaction list. We discuss the optimal choice for the population of bunches in section 7.3.1.

Due to the differently tuned traversal, and because GRAPE processors can compute force interactions to monopole order only, the accuracy of the forces that result from the calculations will be different from those obtained from a tree based solution alone, given the same setting of the MAC. To obtain forces of comparable accu-

racy, the MAC setting must also be modified, to a more restrictive value. In section 7.2.2 we define the MAC settings that produce comparable accuracy for the tree/host and tree/GRAPE modes.

6. OVERVIEW OF THE CODE

VINE is written in the Fortran 95 language, but in a largely Fortran 77 style which will be familiar to and comfortable for most astrophysicists. For this reason, relatively little use has been made of the newer language revision’s features, such as derived types (somewhat similar to C ‘structures’) or pointers. On the other hand, extensive use has been made of the ‘module’ format of grouping procedures together both to improve modularity of the code and in order to enable the improved debugging features such as argument checking available when they are used. The code includes a number of pre-built sub-makefiles for common commercial and open source compilers, which can be selected by the user and each of which contain compiler options grouped by the designations ‘FAST’ and ‘DEBUG’. Sub-makefiles for other compilers we have not included may easily be created by users, using one of the existing files as a template. Although we have made no specific tests to determine an ideal set of options for VINE for any single compiler (other than to note a factor of several difference in speed between the two categories just mentioned), we believe the options selected in each sub-makefile will provide near optimal performance in terms of either VINE’s overall performance or the ease with which it may be debugged or otherwise analyzed for coding errors.

Although some care has been taken to limit the memory footprint of the code, we have not made it a primary focus in our development. Instead, we have concentrated on performance improvements and on reducing the vulnerability of the calculations to errors associated with loss of precision when, e.g., when two quite similar values are differenced, or two quite different values are summed. Errors of this sort will inevitably develop in large simulations because particles are closely spaced and the precision of numerical representation of their positions is finite. In this context, and with an expectation of simulations of ever increasing size in the future, we have made the default size for all real variables in VINE ‘double precision’ (8 bytes on most systems), for which about 15 digits of precision are retained at the cost of doubling the required memory relative to single precision. While even this level of precision does not eliminate finite precision errors, they will at least be of much lower magnitude. In keeping with our philosophy of keeping VINE as modular and adaptable as possible however, VINE’s build system recognizes an option to change the default to single precision values, to permit VINE to be used in constrained memory environments or for extremely large simulations, at or near the capacity of the machine available to its users.

Table 1 contains a listing of all real and integer arrays, normalized to the total number of particles of all types, N_p , and the number of SPH particles, N_{SPH} , and broken down for each component of the code. The number of arrays allocated to the tree actually defines an equivalent number of N_p length arrays because the arrays in the tree hold $2N_p - 1$ elements corresponding to both particles and nodes. The number of arrays is also depen-

dent on the number of dimensions, d , defined at compile time to be either two or three. In typical operation, we expect that the code will include one integrator, use individual time steps, and include gravity using the multipole summation method and the tree. In this case, the total amount of memory required for a simulation containing N_p particles, of which N_{SPH} are also SPH particles will be

$$M = [(d + 20 + 5N_{\text{proc}})I + (13d + 6)D]N_p + [2I + 17D]N_{\text{SPH}} \quad (11)$$

when the leapfrog integrator is used or

$$M = [(d + 20 + 5N_{\text{proc}})I + (15d + 6)D]N_p + [2I + 22D]N_{\text{SPH}} \quad (12)$$

when the Runge-Kutta integrator is used. If double precision values require eight bytes and integers require four, then a 3 dimensional simulation on one processor, with either entirely N -body or entirely SPH particles will require 474 or 584 bytes of memory per particle when the leapfrog integrator is used (292 or 368 bytes in single precision), and 522 or 706 bytes per particle when the Runge-Kutta integrator is used (318 or 410 bytes in single precision). In comparison, VINE requires 30-50% more total memory per particle than the Gadget and GOTPM codes (Springel 2005; Dubinski et al. 2003), when they are used in double precision mode. Approximately half of the extra cost is due to fact that VINE includes the quadrupole in the multipole summation of gravity, which requires 96 bytes/particle to store the quadrupole moments for all nodes. Other important components of memory usage are accounted for by additional arrays used to implement optimizations, allow for modularity or to implement features not present in other codes.

For simulations in which machine memory is a significant constraint, we believe that an optimized version of the code could be developed with a much reduced memory footprint, at the cost of some increased computation. For example, gravitational force calculations might instead be truncated at monopole order rather than quadrupole order, or a number of temporary arrays throughout the code could be deleted in favor of recalculation. Particularly in very high resolution simulations however, we are reluctant to recommend reducing floating point numbers to single precision, even though it provides a factor of two footprint reduction for real values, because of the prevalence of difference calculations in both the gravity and SPH calculations. At very high resolution, or when particles lie close together in space, errors in position difference calculations can grow large simply because the particles share all but the last few digits of their coordinate values. In such cases, and over many calculations, catastrophic cancellation can grow to levels important for correctly realizing the evolution in a given problem Goldberg (1991). Though ultimately impossible to eliminate entirely, we have attempted to design VINE so as to reduce such problems for its users.

7. PERFORMANCE

After describing the code, its features and optimizations, we move now to a discussion of its performance. Two separate qualities of the code affect the performance. First, the code itself has a number of compile

time and run time settings that affect its speed and accuracy, such as the maximum number of particles contained in a clump or the specific MAC used or, at a deeper level, the different optimizations made to the layout of variables in memory as discussed above. Second, the hardware architecture on which the code is run may be faster or slower than some other competing architecture, or may have settings which can be tuned to provide better performance for the code.

In this section, we investigate the sensitivity of calculations with VINE to the settings of a number of parameters, both in terms of the speed and of the accuracy of the calculations. We first describe the initial conditions of three test problems on which we run our tests. Second, we describe the results of tests designed to determine optimal settings for the gravity calculations performed using each of the three multipole acceptance criteria defined in VINE, with and without the use of GRAPE hardware. Next, we explore the sensitivity of the gravity and SPH calculations rates to the size of the clumps used to accelerate the tree traversals. Finally, we describe the serial and parallel performance of the major components of the code and their sensitivity to the various optimizations discussed above.

Our preliminary testing showed that some parameter settings (e.g. high accuracy settings for the MAC used in the gravity calculation) could result in significant impacts on performance as a function of processor count due to limitations such as memory latencies due to NUMA architectures. Although in the end, we found that the most desirable parameter settings do not appear to be highly sensitive to such architectural features, we chose to sample the range of processor counts relatively densely in order to explore sensitivity to such issues. Dense sampling also enables more direct comparisons on several different architectures which may have both different maximum processor counts and different scaling as a function of processor count.

In each of the comparisons that follow, we show the effect of varying one of the parameters to which the code's speed is sensitive, while keeping all others fixed at their optimal values. For reference, and unless otherwise indicated, we run the tests using 8 processors of the Origin 3000 listed in table 3 and we use the Gadget MAC with an opening criterion set to $\theta = 5 \times 10^{-3}$. This setting yields gravitational forces for 99% of particles that are accurate to a few $\times 10^{-3}$, as we show in section 7.3. We use a maximum population of 70 particles in a single clump and we trigger a complete tree rebuild when the size of any clump reaches twice its value immediately following the rebuild. We use cache blocking, tuned to the size of the L1 cache of each architecture⁷, and the largest page size available on each machine. Finally, we reorder the particles before performing any of the speed tests. In these tests, one 'calculation of SPH quantities' is dominated primarily by the calculations of the mass density and the hydrodynamic forces. It also includes the calculation of the equation of state, the internal energy derivative, and smoothing length variation.

⁷ Note however that Itanium 2 processors permit only integers to be loaded into the L1 cache, so for that architecture, we use cache blocking tuned to the size of the L2 cache

TABLE 1
NUMBER OF ARRAYS REQUIRED BY VINE MODULES

Module	Integer	Double	Integer (sph)	Double (sph)
Particle data	2	$4d + 5$	1	8
Integrator data				
Leapfrog	0	d	0	3
Runge-Kutta	0	$3d$	0	8
Ind. TS data	6	2	0	0
SPH data	0	0	1	6
Force law data	0	$6d - 6$	0	0
Tree data	11	$2d + 5$	0	0
Tree build runtime	$1.0N_{proc} + d$	0	0	0
Tree runtime	$4.5N_{proc}$	0	0	0
Pnt. Mass runtime	1	0	0	0
Grape 6 data	0	10	0	0

7.1. Description of the test problems

Because the code can be used to follow the evolution of N -body particles alone, SPH particles alone, or both together, we will define a test problem for each option, in order to demonstrate its performance in each kind of simulation. These three test problems will be referred to as the N -body test problem, the SPH test problem and the mixed test problem. In order to understand the performance of the code as a function of resolution, the mixed problem will have realizations at several resolutions.

7.1.1. The N -body test problem

The N -body test problem is a sphere with density profile of $\rho \sim R^{-1/4}$ which is set up according to the method described by (Hernquist 1990a) and which is realized with 7×10^6 particles. A lower resolution version with 2×10^6 has been used for the force accuracy tests in section 7.2.1. Our system has a total mass of $5.6 \times 10^{12} M_\odot$, a cut off radius of 175 kpc and a scale radius of 35 kpc. We also consider variants of this test with particle counts ranging to as low as 160000 (see table 2), in order to study the influence of resolution on bunch size (section 7.3.1) and force accuracy when GRAPE co-processors are used. For all tests involving the GRAPE processors, or comparing the speed of VINE to them, we employ Plummer softening, while all other measurements involving these tests we use the fixed spline softening option. In order to maintain systematically consistent timings at different resolutions, we scale the gravitational softening length according to the cube root of the number of particles in the simulation.

7.1.2. The SPH test problem

The SPH test problem is a set of two conditions defining the initial and evolved state of a turbulent molecular cloud which undergoes fragmentation and forms stars. It is identical in setup to the simulations of Bate et al. (2003), however it was set up using a different random seed. The molecular cloud in this model is initially spherical, with uniform density and is realized with 3.5×10^6 particles. It has mass and diameter of $50 M_\odot$ and 0.375 pc respectively, and it has an initial temperature of 10 K. The free-fall time of the cloud is $t_{ff} = 1.9 \times 10^5$ yr and the late time condition has undergone slightly more than one free fall time of evolution and is characterized by a very inhomogeneous density distribution. For more details, we refer the reader to Bate et al. (2003).

7.1.3. The mixed test problem

In order to test the code's abilities on a problem which incorporates both N -body and SPH particles, we use a set of initial conditions for spiral galaxy mergers, similar to those used by Naab et al. (2006b) and Wetzstein et al. (2007), in which two spiral galaxies are initiated on a parabolic orbit at a distance of 105 kpc. Each galaxy consists of a stellar disk and bulge, a gaseous disk and a dark matter halo, set up according to the method of Hernquist (1993). The components have masses of $M_d = 3.92 \times 10^{10} M_\odot$ and $M_g = 1.68 \times 10^{10} M_\odot$ for the stellar and gas disks respectively, and $M_b = 0.2 M_d$ for the stellar bulge and an additional mass of $M_h = 3.248 \times 10^{10} M_\odot$ defining the dark matter halo. Both stellar and gas disc have an exponential surface density profile with scale lengths of 3.5 kpc and 10.5 kpc, respectively. The dark matter halo is modeled as a pseudo-isothermal sphere with a core radius of $r_{c,h} = 3.5$ kpc and a cut off radius of $r_{cut,h} = 35$ kpc. For more details about the initial conditions, we refer the reader to Wetzstein et al. (2007).

We have created models of this merger setup at six different resolutions (see table 2). In the lowest resolution model, Merger1, each galaxy contained 37500 particles for the stellar disk, 18750 for the gas disk, 3750 for the stellar bulge and 75000 for the dark matter halo. For each higher resolution model in the sequence, the particle numbers of each species have been doubled. The fraction of gas particles, for which SPH calculations are required, thus remains constant for each resolution at $\sim 14\%$ of the total. Due both to this comparatively small fraction, and the inhomogeneous spatial distribution, this problem will therefore represent a challenging test of the load balancing and parallel efficiency achievable by the calculations of the hydrodynamic quantities with SPH.

7.2. Tuning the code I: accuracy and speed of various alternatives for the gravity calculations

The ability to compute forces accurately enough to integrate particle trajectories correctly using a tree based force calculation is governed by the choice of the MAC and its setting. In this section we present quantitative tests of the accuracies for all three opening criteria implemented in VINE: the geometric MAC (equation 7), the SW absolute error MAC (equation 8) and the Gadget MAC (equation 9).

We perform our tests on low and high resolution versions of our N -body test problem, as well as the initial

TABLE 2
TEST SIMULATIONS

Name	Number of SPH Particles	Number of N -body Particles
N -body 1	0	160000
N -body 2	0	320000
N -body 3	0	640000
N -body 4	0	2000000
N -body 5	0	7000000
SPH (Initial)	3500000	0
SPH (Evolved)	3500000	0
Merger1	37500	232500
Merger2	75000	465000
Merger3	150000	930000
Merger4	300000	1860000
Merger5	600000	3720000
Merger6	1200000	7440000

and evolved states of our SPH test problem. The low resolution N -body test was realized with 2×10^6 particles. For all tests with the GRAPE/tree option, a GRAPE-6A board ('MicroGRAPE') has been used.

We determine exact accelerations in each of the test problems using either a calculation of the forces using the direct summation option in VINE, or the geometric MAC with an opening criterion set to $\theta = 10^{-10}$, effectively equivalent to a direct summation of the contributions from each particle on the others. These exact values were used as references to calculate errors in the magnitudes of the accelerations, defined as

$$|\delta \mathbf{a}| = \frac{|\mathbf{a} - \mathbf{a}_0|}{|\mathbf{a}_0|} \quad (13)$$

where \mathbf{a} and \mathbf{a}_0 are the approximated and exact accelerations, respectively.

Determination of a specific limit on the acceptable errors will in general depend on the system simulated, the time span over which the system must be evolved, and the goals of the simulation. Several general principles hold for most systems however. First, it will be desirable to have a narrow error distribution, since the work required to compute highly accurate accelerations on some particles will be wasted if the simulation evolves incorrectly due to much larger errors of others. In general, a reasonable requirement for force accuracy is that the vast majority, say 99%, of the particles have force errors below 0.1–0.5%. In addition, we consider it a reasonable requirement that none of the remaining 1% of particles have errors larger than some other, higher threshold, say 1%. This second condition avoids the possibility that a substantial 'tail' distribution of particles exists and which have very large errors that are large enough to alter a simulation's evolutionary trajectory even though the population is small. Therefore, we will adopt both of these limits in our analysis. Again however, we note that the question of what force error distribution is required for accurate simulation of a given system, depends both on the system morphology, and on the goals of the researcher. The MAC settings required for the code in such cases may therefore be higher or lower than quoted here, though the values we choose are known to work reasonably well on a wide variety of problems in the literature.

Figure 2 shows distributions for each of the three MACs implemented in VINE, for both the tree based calculation and the GRAPE/tree combination, performed

on a single Itanium 2 processor, or in combination with a GRAPE-6A. In sections 7.2.1 and 7.2.2, we discuss these distributions in detail.

7.2.1. Accuracy using the tree/host based calculation

The left panels of figure 2 show the cumulative error distributions for the tree based force computation performed on the host. The most relevant parts of the distributions are the overall widths of the distributions and the upper right part of each curve, which show the population of particles with the largest errors in the calculation. These are the most likely to cause visible numerical errors to the evolution of the system, due to inaccurate integration of particle trajectories.

For the geometric MAC, the distribution rises steeply towards larger errors, through an 'S' shaped curve, with a small 'tail' population at the high end limit of the distribution and a somewhat larger tail population at the low end limit. Though we have made no explicit study of particles in either the high or low error tails, we presume that most near the high error limit are those for which the absolute magnitude of the force is small, so that the relative error is correspondingly larger. For $\theta = 1.0$, the high error tail extends to errors as great as $\sim 0.8\%$ and about 25% of the particles have errors greater than 0.1%, though none have errors as large as 1%. The case of $\theta = 0.8$ produces more accurate results, but still $\approx 4\%$ of the particles have force errors $> 0.1\%$. When $\theta = 0.6$, no particle has errors above 0.1%. This setting produces an error distribution somewhat more restrictive than the requirement we define above, and we conclude that adopting a value of $\theta = 0.6 - 0.7$ in VINE can be regarded as acceptable for most scientific applications.

For the SW MAC, the error curve again follows an 'S' shape, with similar maxima, of $\sim 0.5 - 0.8\%$, for the most permissive settings. Because VINE converts all quantities to dimensionless units for use inside the code, stating a specific value for the SW MAC setting loses meaning, since without details of the unit system in place, limits on the contribution of any given node to the absolute force error become difficult to interpret. Nevertheless, and with the understanding that the unit conversions are done with the intent of converting the relevant physical variables to unit-less quantities near unity, we provide such a statement. For the particle distribution here, a values of $\theta < 0.05 - 0.1$ (in internal code units) appears

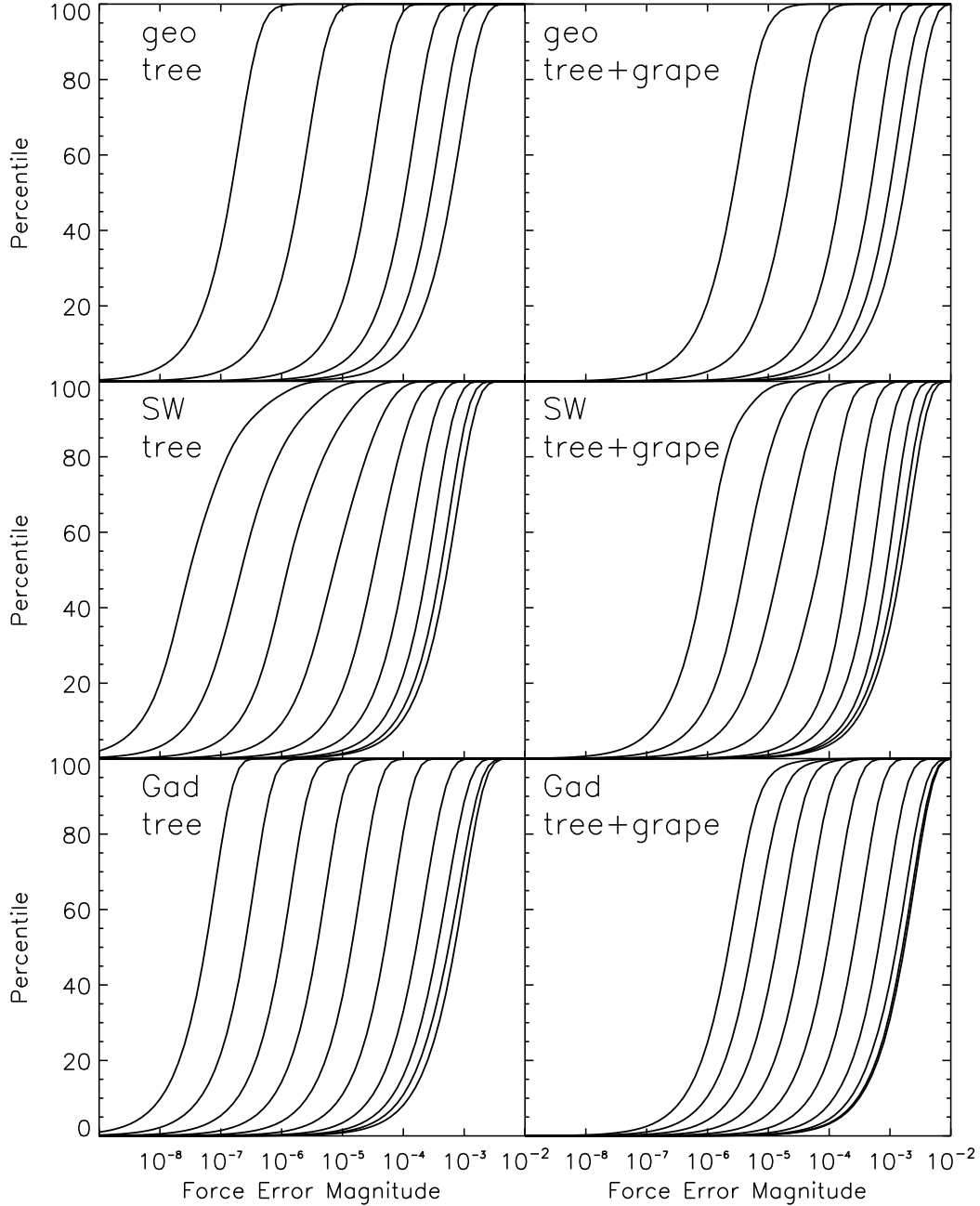


FIG. 2.— Cumulative distribution of the fraction of particles with relative force errors lower than a given value. The left column shows the force error distributions for the tree on host, the right column for the GRAPE-tree combination. Results for the geometric, SW and Gadget MACs are shown in the top, middle and bottom rows, respectively. For the geometric MAC, the curves represent $\theta = (0.1, 0.2, 0.4, 0.6, 0.8, 1.0)$, for the SW MAC curves correspond to settings of $10^{-6} \leq \theta \leq 10^2$ in decade increments and for the Gadget MAC curves corresponding to $10^{-9} \leq \theta \leq 10^0$ in decade increments are shown.

to be acceptable to use if our limit described above is applied. For other unit systems, perhaps implemented by VINE’s users, a different setting may be required.

For the Gadget MAC, the error distributions again rise steeply as a function of error magnitude and, although the largest errors with the most permissive settings extend to slightly larger values than for either of the other two choices, no particles with errors greater than 1% are found for any setting. Settings with $\theta \gtrsim 10^{-2}$ produce unacceptably large errors in the forces according to the criteria above, while values $\theta \lesssim 10^{-3}$ provide more restrictive error limits. We suggest that a reasonable choice is $\theta \sim 1 - 5 \times 10^{-3}$, to approximate our chosen error cri-

teria.

An important characteristic of the geometric and Gadget MACs is that the shape of the error distribution is both narrow and changes little as the tolerance parameter, θ , decreases, so that the curve simply shifts further and further to the right. This is a very desirable feature not only because errors for the majority of particles decreases, but also because the largest force errors are effectively controlled by reducing θ . If instead a significant population of particles remain with large errors, while the rest decrease, a simulation may become computationally costly while remaining insufficiently accurate. This is because particles whose forces errors are large can

affect the evolutionary trajectory of a simulation disproportionately to their number (for a particularly dramatic example of such effects, see e.g., the exploding galaxy problem in Salmon & Warren 1994), so controlling their behavior is of particular importance for accurate simulations.

In contrast, while the error curves for the SW MAC for the most permissive tolerance settings appear very similar to those of the other two, curves representing more restrictive settings do not. The distribution shifts not only towards lower errors, but also changes shape. While the low end of the distribution decreases steadily, the high error tail does not, leading to a large spread in the calculated error magnitudes for different particles. We believe the widened distribution is a consequence of the fact that the SW MAC, as implemented in VINE, constrains the absolute error magnitude of the force on each particle, while figure 2 shows relative error magnitudes. In a system where particles have a wide distribution of force magnitudes, errors for particles with small magnitudes will decrease less quickly than those with larger until the opening criterion falls to some critical value for a given particle and causes additional nodes to be opened in the tree.

Finally, we note that for the most permissive settings of both the SW and Gadget MACs, and for the same relative change in the MAC setting, much smaller differences are seen in the error distributions compared to changes at more restrictive settings. This is an important feature of both MACs because they imply an effective upper limit on the force errors, a clearly desirable feature for numerical realization of any physical system, all the more so since the error limits remain comparatively small.

We believe the reason for the limit is that both MACs enforce a requirement that tree nodes are only accepted for use in the force summation if the particle (or clump) on which forces are calculated lies exterior to the node itself (see Vine1, section 4.2) for any setting of the MAC. This physical constraint corresponds to the numerical condition that a given tree traversal will produce the shortest possible list of acceptable nodes for use in the force summation, for that MAC. The most permissive settings shown in figure 2 have clearly entered the regime where convergence of the generated interaction list towards this minimal list has begun, and implying that the error limits shown are near those of the minimal list as well. The geometric MAC does not explicitly contain a similar condition, however the same effect is still realized in practice because source and sink nodes may overlap in space for settings with $\theta > 1$, a condition which violates the assumptions underlying the multipole approximation used to approximate the forces in the first place. For a more detailed discussion of this effect, we refer the reader to section 7.2.3.

7.2.2. Accuracy of the GRAPE/tree combination

Error distributions for the GRAPE-tree based force calculations are shown in the right panels of figure 2. As expected for calculations involving GRAPE hardware, errors for all three MACs are larger than in the corresponding tree/host based calculation for identical MAC settings. Except for the most permissive tolerance settings, error limits an order of magnitude larger are typically realized with the GRAPE/tree option in compari-

son to those with the tree/host option. While maximum errors remain below $\sim 1\%$, more restrictive settings do not shift to smaller errors to nearly the extent that the tree/host based calculations do, for the same tolerance parameter.

We interpret each of the effects as consequences of the differences between the code implementation in either case. The GRAPE/tree combination makes use of a modified tree traversal (section 5.3), with large clump sizes ('bunches') for the far traversal and does not terminate with a list of neighbor bunches for use in a close traversal, but instead calculates many more pairwise interactions between individual particles. This feature implies a more accurate calculation of the forces from nearby particles on each other. At the same time however, the GRAPE/tree option accounts only for the monopole moment of a node, and so implies a less accurate calculation of forces from more distant particle groupings. Therefore, for the same value of the tolerance parameter θ , the computed accelerations are less accurate than those of the tree based calculation, which includes quadrupole moments too.

For this problem, error limits at or below the constraints defined above remain within reach of the GRAPE-6A/tree combination, but require much more restrictive settings of the opening criterion. Values of the opening criterion of $\theta \lesssim 0.6$, $\theta \lesssim 10^{-2} - 10^{-3}$ and $\theta \lesssim 10^{-4} - 10^{-5}$ are required for the geometric, SW absolute and Gadget MACs respectively.

7.2.3. The relative speed of using different MACs for a given accuracy

In this section, we examine the relative efficiency of using each MAC for producing accelerations of a given accuracy. For these tests, we use the full N -body test problem and both variants of the SPH test problem. Each test uses the same executable code, running on 8 processors of the Origin 3000. For each run, we specify the MAC and MAC setting via an input file, run the executable and output accelerations for all the particles for later analysis. We sort the errors according to their magnitude to determine the value of the error magnitudes below which 50% and 99% of particles lie. Combining information from both error limits, it will be possible to quantify both an approximate upper limit on the errors and a crude measure of the overall width of the distribution, from the difference between the two quantities. The overall shapes of the error distributions are similar to those shown in figure 2.

Figure 3 shows the rate of gravity calculations per second as a function of the 50% (i.e. median) and 99% error magnitudes. In their asymptotic, high accuracy limits, the rates for each MAC are each approximately proportional to the square of the accuracy. This proportionality is expected from the truncation of the multipole series at quadrupole order (Salmon & Warren 1994). In that limit however, the Gadget MAC yields rates that are a factor ~ 2 higher than those of the geometric MAC, with the SW MAC lying between and yielding a slightly different proportionality. The difference appears to be due to the fact that the SW MAC is used in its form as a limiter on the absolute error magnitude that any given node can contribute rather than the relative error, as is the case for the other two MACs. We attribute the overall speed

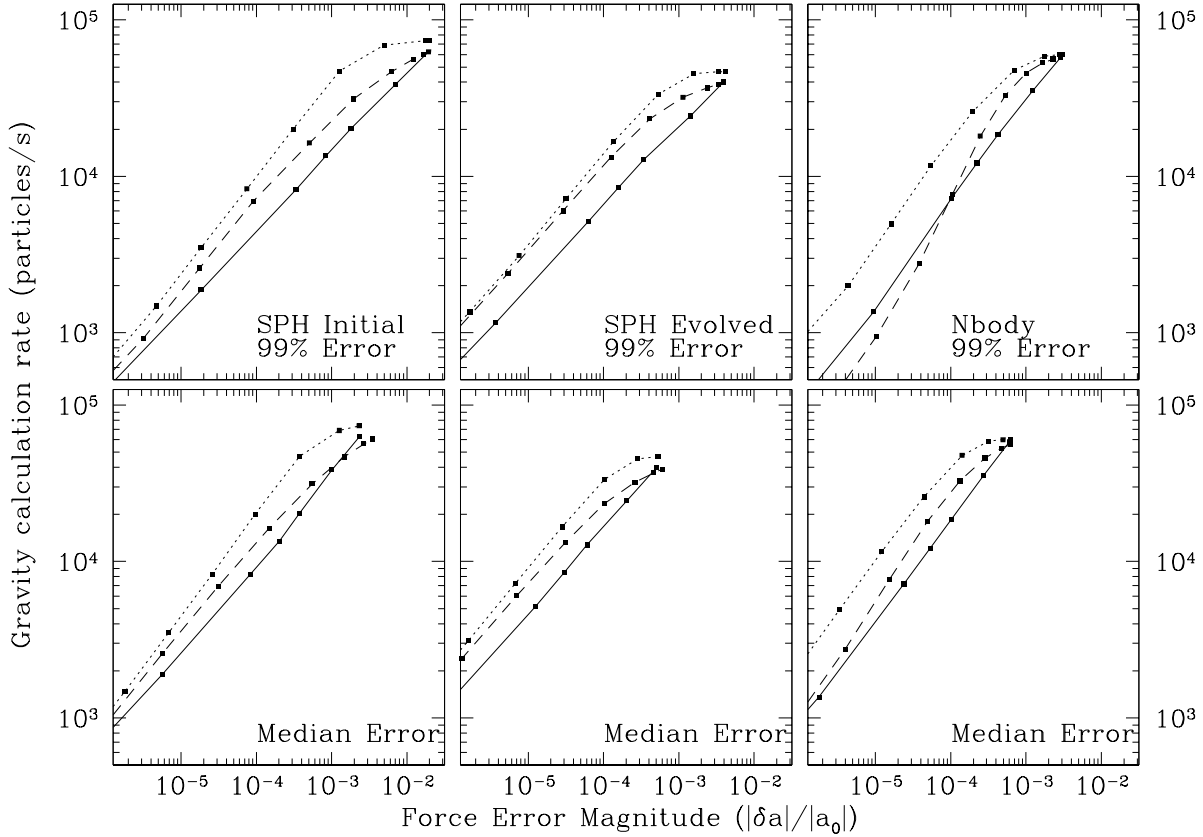


FIG. 3.— The rate of gravitational force calculations for the code using the three MACs implemented in VINE, as a function of the accuracy. The top panel shows the rates for which 99% of the particles have error magnitudes less than that shown, while the bottom panel shows the rates for the median error rate, at which 50% of particles have error magnitudes less than that shown. The solid curve shows the rates obtained from the geometric MAC, the dotted curve shows the rates from the Gadget MAC and the dashed curve shows rates for the SW MAC. Points correspond to settings of $\theta = 0.1, 0.2, 0.4, 0.5, 0.6, 0.8$ and 1.0 for the geometric MAC, to settings of θ in decade increments from 10^{-8} to 10^0 for the Gadget MAC, and to settings θ in decade increments from 10^{-6} to 10^2 for the SW absolute error MAC, using internal code units for the forces.

differences between the MACs to the fact that while the geometric MAC accounts for only the physical size of a source node, each of the other two also account, in different approximations, for its internal structure as well. The additional information proves valuable in allowing nodes to be selected, which otherwise would need to be opened and examined in more detail.

The error magnitudes for the most liberal settings of each of the three MACs in the same test vary only slightly from one another. The similarities are presumably due to the fact that the three different opening criteria each reduce to the same physical condition that the sink point at which the force is calculated must be exterior to the source node that exerts the force. Although the error magnitudes from the same test are similar, they differ from one particle distribution to the next, as do the calculation rates realized for those errors. The rates are highest in the case of the SPH initial condition and lowest for the evolved condition, with the Hernquist sphere lying in between. The differences are significant because we expect that the speed of a gravitational force calculation will be proportional to $N_p \log N_p$, and would therefore expect similar rates in the two SPH conditions and lower rates in the N -body test with twice as many particles.

Some clarity emerges if we also correlate the rates and relative force errors in each problem and their overall morphology. The relative force errors are largest in the SPH initial condition, smallest in the evolved condition and intermediate in the Hernquist sphere—an opposite trend from that seen for the rates. At the same time, while the SPH initial condition is quite smooth, the Hernquist sphere is centrally condensed and the evolved SPH condition is near the onset of fragmentation and is even more inhomogeneous. We therefore attribute the rate and accuracy differences to the differences in particle distributions in each test and conclude that, at least on scales of factors of two difference in particle count, the morphology of the particle distribution plays a role much larger than the overall scaling.

Even for the most liberal MAC settings, the median and 99% error magnitudes are well below 1% and $\sim 2\%$ respectively for all three MACs for smooth conditions, and nearer to $\sim 0.5\%$ for the same settings in non-smooth conditions. This level of precision differs from the behavior of many other codes, given the same MAC and setting (see, eg., corresponding figures in Springel et al. 2001; Springel 2005; Wadsley et al. 2004; Dubinski et al. 2003), first, because the calculated size of each node (equation 5) as incorporated into the MAC for that node

is always an overestimate of its true size, so that a search will tend to open more nodes than are strictly required. Second, dividing the traversals into far and near components for groups of particles means that, for a given setting, more nodes and atoms are required than would be the case for a single particle. While the MAC must be satisfied for every node on the interaction list at the point in the clump closest to that node, most particles in the clump will be found further away, where the node's parent might otherwise be acceptable. The trade off is beneficial in the sense that fewer traversals are required, even though more interactions result.

Of particular interest for most numerical simulations is the range of relative errors above a few $\times 10^{-4}$. In this range, the additional information describing the internal node structure and incorporated into the Gadget and SW MACs provides its greatest benefit. The rates obtained from the Gadget MAC decrease from their most liberal settings by only $\sim 20\%$ while the calculation becomes an order of magnitude more accurate, and the setting itself changes from 10^0 to 10^{-3} . The SW MAC exhibits a similar, but less pronounced characteristic.

Given the results of these tests and those of the previous sections, we recommend the use of the Gadget MAC in VINE, with a setting of $\sim 5 \times 10^{-3}$, for simulations to run at both high accuracy and high efficiency. This setting ensures maximum relative errors of $\sim 1\%$ in very smooth conditions, and $\sim 0.1 - 0.2\%$ in more evolved systems, without increasing the cost of the calculation. This accuracy is also comparable to the expected numerical noise present in the hydrodynamic quantities of SPH simulations (Herant & Woosley 1994), below which higher accuracy will yield little additional benefit to a simulation.

7.3. Tuning the code II: optimal software settings and memory layout optimizations

In this section, we will discuss the performance of the most costly components of simulations using VINE that interact with the tree. In order, these are the gravity calculation, the SPH calculations and the tree build/revision. We explore the sensitivity of the performance to various optimizations, in order to quantify the influence that each makes on the total absolute performance and the scaled performance. For our purposes, absolute ('raw') performance will be defined simply by higher calculation rates, while scaled performance will be defined by efficiency of parallel scaling, relative to the performance on one processor.

7.3.1. The optimum number of particles in a clump or bunch

The tree traversal strategies described in sections 4.2 and 5.3 each contain one free parameter that must be tuned in order to provide the best performance, namely the number of particles contained in a clump or bunch. In the case of clump population, both the gravity and the SPH calculations will be affected because tree traversals are done in both cases, to search for acceptable nodes and atoms in the gravity calculation, or for neighbors in the SPH calculations.

Clumps and bunches may be populated by any number of particles up to and including a preset maximum. In this section, we explore the sensitivity of the calculation rate to that maximum population value. We choose

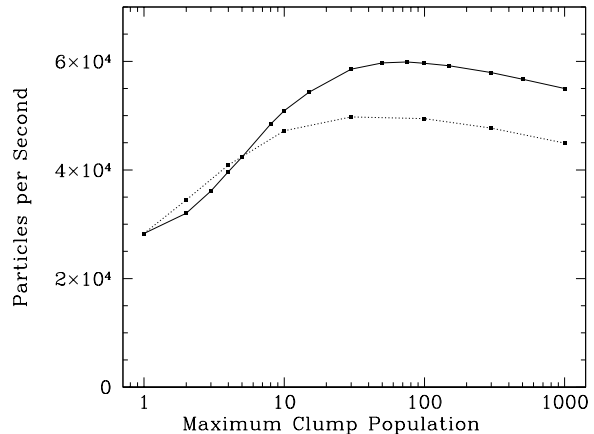


FIG. 4.— The calculation rate for gravitational forces on particles in the N -body test problem, as a function of the maximum particle population in a clump. The solid curve shows the rates with cache blocking, while the dotted curve shows the rates without. Both use the Gadget MAC, with opening criterion $\theta = 5 \times 10^{-3}$.

the maximum as our metric because it is easily available for modification by the user, while the more directly intuitive values of average or exact populations must be derived from the particle distribution and the exact tree structure. Over a wide variety of morphologies, we have found that the population distribution fills essentially all values from 'singleton' clumps up to the maximum, and the average fall typically at $\sim 50 - 60\%$ of the maximum.

Figure 4 shows the calculation rates for a single gravity calculation with the N -body test problem as a function of the maximum number of particles contained in a clump. As the maximum is increased from a single particle to ~ 30 , the calculation rate increases by a factor of ~ 2 . Increasing the maximum further results in much smaller improvements, with a broad maximum in the rates near ~ 70 particles per clump. Relative to the performance with a clump population of one (i.e. individual traversals for each particle), we obtain a speedup of ~ 2.1 . The two curves represent the performance obtained with and without cache blocking (see section 5.1), and while both versions show improvements over the rate for individual traversals, the unblocked version does not increase nearly as much, saturating at a factor ~ 1.75 . The differences are important to quantify because when individual time steps are used in a simulation, only a relatively small fraction of the particles in a clump will be active. In this case, the benefits from cache blocking will be reduced by a factor related to the fraction of active particles in each clump, and will more closely reflect the rates without cache blocking. Even in the case when only two particles are active in a given clump, some benefit of the cache blocking is retained however, so we enable it by default, except when only a single particle is active in a clump.

Figure 5 shows calculation rates for a single calculation of all SPH quantities, including both densities and the hydrodynamic accelerations, using the initial and evolved particle distributions in the SPH test problems described above. Here again we see a substantial improvement as the maximum clump population increases. In the case of the initial condition, the rate increases by a factor ~ 1.5 over that required for clumps defined as single particles. The evolved state speeds up by a much greater factor of ~ 3 , presumably due to an increased level of data

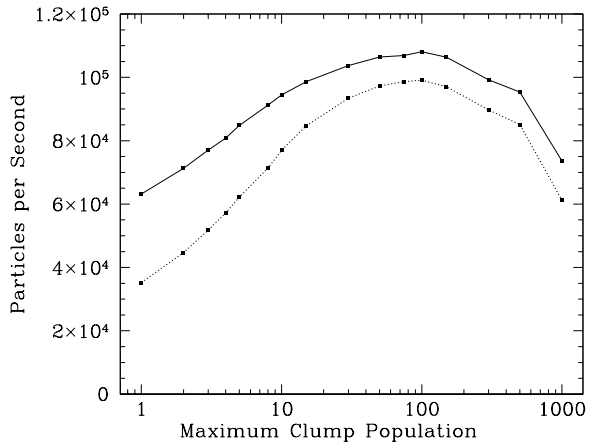


FIG. 5.— The rate that all SPH calculations required in the two SPH test problems can be calculated, as a function of the maximum number of particles in a clump. The solid curve represents the times for the initial condition, and the dotted line represents the times for the evolved state.

reuse when calculations for nearby clumps occur in close succession. Even for the fastest setting, the time required for the evolved particle distribution does not match that of the initial state however, where the optimal rate is about 10% higher. We have not attempted to trace the difference to a specific cause, however it is comforting to realize that in spite of the quite different morphologies, the rate of calculation changes by only a relatively small amount.

For both the gravity and the SPH calculations, the maximum rate occurs when the maximum number of particles per clump is $\sim 50 - 70$. We have therefore chosen to set its default value in VINE to 70 in 3D simulations, which is also the setting for the maximum number of neighbors allowed for any SPH particle, before limiters are activated which push the number downwards again (see additional discussion of these limiters in Vine1). No detailed tests have been performed to determine an optimal setting for 2D simulations, however small scale tests (not shown here) indicate that the optimal value is smaller. As for 3D, we set the maximum to the maximum number of SPH neighbors, which is ~ 30 for 2D simulations.

The speed of the gravity calculation is also sensitive to the clump population when the tree is used in combination with the GRAPE hardware. So much so that it even lead us to define a different, larger grouping (‘bunches’) for use in combination with GRAPEs, as discussed section 5.3. The reason for the sensitivity is more complicated when GRAPE is used however because the time to solution includes contributions from not only tree traversal and multipole summation computation, but also from communication to and from the GRAPE processor.

Figure 6 shows calculation rates for a single gravity calculation of the N -body test problem as a function of maximum bunch population and using VINE in GRAPE+tree mode, and for a number of resolutions. We use the Gadget MAC with $\theta = 5 \times 10^{-3}$ for all tests and include one comparison to the geometric MAC with $\theta = 0.75$ for the case with 640000 particles. As was the case for clump populations in the the host-alone gravity calculation, the calculation rate is sensitive to the maximum bunch population. The peak rates increase by a

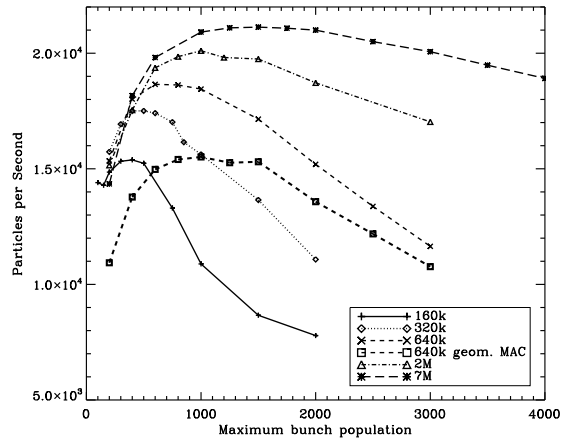


FIG. 6.— The calculation rate for gravitational forces on particles in the N -body test problem at several resolutions, as a function of the maximum particle population in a bunch. We use the Gadget MAC, with opening criterion $\theta = 5 \times 10^{-3}$. For comparison, one test with the geometric MAC and $\theta = 0.75$ is shown as well. The host was a single Itanium2 processor and used a GRAPE-6A (‘MicroGRAPE’) board for the gravity calculations themselves.

factor of ~ 1.5 or more over those for smaller or larger populations. Of interest is the fact that the optimal bunch population changes as a function of the resolution of the simulation itself, even though the simulations are of identical configurations. While the case with 160000 particles has an optimal maximum bunch population of $\sim 400 - 600$, the optimal population for the 7×10^6 particle realization is near $\sim 1200 - 1800$. Because the calculation speeds change little over a fairly broad plateau of maximum bunch populations, it is easy to achieve a near-optimal choice even without extensive testing. The calculation rate decreases much more steeply for bunch sizes lower than the optimum than for bunch sizes greater than the optimum, so it is safer to adopt a higher value if an estimate is required.

We believe that the sensitivity is a consequence of the fact that the physical size of a bunch containing a given number of particles decreases as a function of increasing resolution, but the MAC remains the same. This is important because the preliminary interaction list for a bunch (i.e. the interaction list that does not include the bunch members themselves), will contain a volume just outside its boundary in which most interactions are with particles, rather than with nodes. If that volume is determined by the MAC setting, through appropriate choices as to which nodes to open or accept, then much more time must be spent in portions of the tree traversal that open all nodes to their fullest extent—an inefficient use of resources. If instead, we assume that bunches contain more particles, a large fraction of such tree nodes will be resolved at the level of single particles by assumption, so that all costs of tree traversal for this volume will be removed. Taking the argument to the extreme however—allowing only a single bunch with all of the particles so that the calculation returns to a pure $O(N_p^2)$ proportionality—illustrates that there is clearly a point of diminishing returns where this argument fails.

7.3.2. Performance of the gravity calculation and the effects of memory layout optimizations

In this section, we turn to a discussion of the serial and parallel performance of the gravitational force cal-

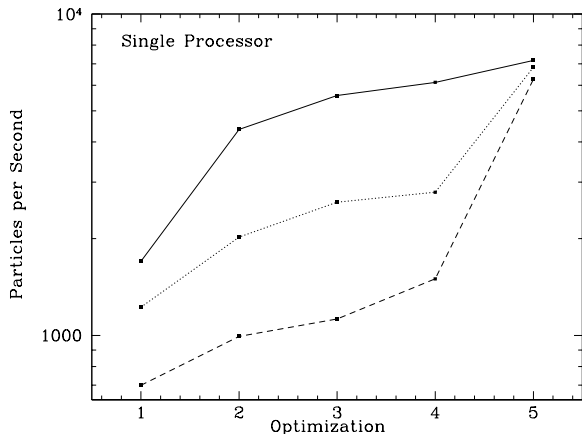


FIG. 7.— The rate that gravitational forces on particles in the N -body test problem can be calculated on one processor under cumulatively more memory layout optimizations, as defined in the text. The three curves represent the rates obtained using hardware page sizes of 16MB (solid), 1MB (dotted) and 64kB (dashed) that are available on the Origin 3000.

culuation, which will typically be the most costly part of any particle simulation of a self gravitating system. We also discuss the benefits of each of the memory layout optimizations discussed in sections 2.4 and 5.1. For these tests, we use the N -body test problem.

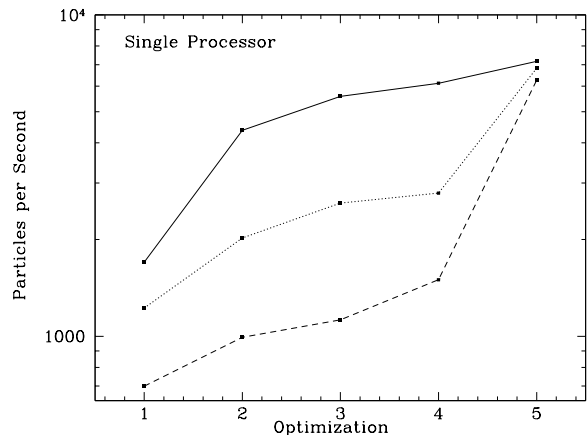
In figure 7, we show the speed of a single gravity calculation performed several times with a different set of optimizations: each realization contains all optimizations of the previous levels, and one addition. Defined as in the figure, optimization level one means that no optimizations are employed, other than to use the Gadget MAC. Tree traversals are done for individual particles, all node data are stored in separate arrays and are not reordered as discussed in section 3.5. For level two, traversals are done on clumps rather than single particles and for level three, the tree data are reordered to reflect the order of access in the traversal. Level four arranges node data in two dimensional arrays so that all data for a single node are located together in memory. Finally, level five implements the cache blocking optimization. Although not dependent on any specific code change, the setting of the hardware page size defines an additional ‘level’ of optimization which influences calculation speed. To determine the effects that it may have on the code, we repeat each test for each of three page sizes: 64kB, 1MB and 16MB.

For the completely unoptimized case, serial performance is 700, 1225 and 1700 particles per second for the small, medium and large page sizes respectively. With all optimizations included, the calculation rate increases to 6270, 6830 and 7170 particles/s, for the same page sizes, respectively. Total performance enhancement from the slowest (level one with 64kB page size) to fastest (level 5 with 16MB page size) calculation is a factor ~ 10 , with an additional factor of ~ 2 coming from selection of the Gadget MAC in favor of the geometric MAC as we saw in section 7.2.3. Although each addition results in performance enhancement relative to the previous level, we do not believe that the specific ordering as defined in the figure is required for improvements in the code. Though we have not quantified the contribution of each

optimization in isolation, we expect that each will provide benefits, independent of all others, to any code that implements them.

For all but the highest optimization level, variation between rates of identical optimization but different page sizes is much larger than variation between one optimization level and another with the same page size. Moreover, identical optimizations provide different performance enhancements when different page sizes are used. For large pages, moving to grouped tree traversals provides more than a factor three speedup, far more benefit than any of the other optimizations. For small pages, the total speedup provided by the first four optimizations together provides only a factor two benefit, with a further benefit of a factor of four from cache blocking. We believe that while the exact source of the variations is unimportant, they are most likely due to the relative costs and frequencies of simply loading a value from cache or memory compared to that of computing a new TLB entry.

In terms of the ‘FLOP’ rate (floating point operations per second) achieved by the code, we have profiled tests similar to these with the ‘perfex’ utility available on Origin 3000 systems. We found that the code achieves approximately 400 MFlops per second, or about half of the theoretical maximum of 2 flops per clock cycle for 400MHz R12000 chips. We believe this rate is near ‘perfect’ in the sense that the mix of operations (i.e. the proportion of adds and multiplies) in most computationally intensive loop (summing the multiple contributions from nodes), is able to utilize only some 60% of the possible operations and the tree traversal portion of the calculation contributes almost no floating operations to the total.



In figure 8, we show the speed of a single gravity calculation as a function of the number of processors for the same series of optimizations described above. For the unoptimized version, parallel performance increases near linearly up to a maximum of only 10 processors and saturates entirely at a speedup of ~ 15 . As for single processor performance, absolute performance is better with larger pages and, for successively higher optimization levels, raw performance continues to increase faster for large page size runs than for small. While providing superior absolute performance at all processor counts, parallel scaling performance with large page sizes saturates on fewer processors. We believe the reason can be tied to the fact that the NUMA related latencies for ob-

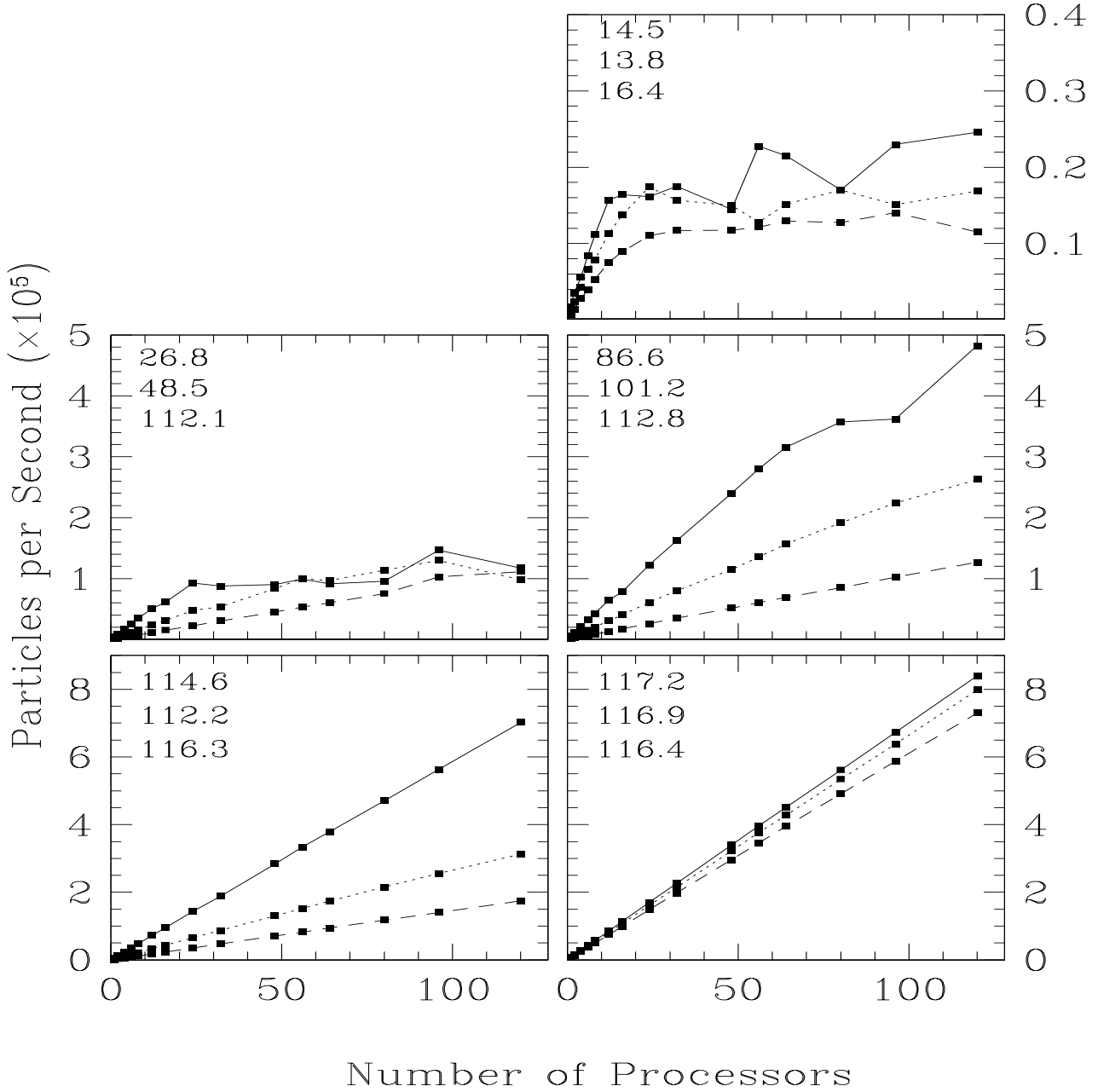


FIG. 8.— The rate that gravitational forces on particles in the N -body test problem can be calculated under cumulatively more memory layout optimizations, as discussed in the text. Each panel contains three curves representing the rates obtained using hardware page sizes of 16MB (solid), 1MB (dotted) and 64kB (dashed) that are available on the Origin 3000, as a function of number of processors. Top to bottom, the numbers in the upper left corner of each panel are the scaled parallel speedup of the code for the 16MB, 1MB and 64kB page sizes, respectively, out of a maximum of 120 for linear speedup. Note that the vertical scale at each of the three panel levels are larger in the lower panels.

taining data from distant nodes are partly masked by the times required to calculate new page addresses. When fewer TLB entries are required, only the NUMA latencies remain.

For the two highest optimization levels, scaled performance for all variants is only slightly below the ‘perfect’ scaling obtained by dividing the single processor time by the number of processors. Raw performance is dramatically different, with only the cache blocking optimization providing performance that is largely indepen-

dent of page size. The discrepancy between scaled and raw performance is important to note because while better scaled performance is desirable, it is actually better raw performance that increases scientific productivity. A code that scales linearly to a large processor count may in fact perform less well than another that does not scale as well, but whose speed in an absolute sense is faster. The optimizations described here increase both the raw and scaled performance of the code.

It is also important to note that for the fully optimized

code, only a comparatively small 14% performance deficit for small pages relative to large pages remains. This is important because large hardware pages on most systems are difficult or impossible to use effectively in production environments. Without cache blocking and on systems without adequate support for large pages, rates would otherwise suffer dramatically and simulations will proceed far more slowly. The cache blocking optimization thus ensures a better level of tolerance to limitations of the hardware itself. We believe the differences that remain are unavoidable and a consequence of the fact that, while the force summation can be cache blocked, the tree traversal itself cannot be. Because the tree traversals sample a very large memory space very sparsely, TLB entries must be discarded and recalculated much more frequently when smaller page sizes are used, resulting in slower execution times. The remaining rate difference is small because the traversals require only 10-20% of the total time required for the gravity calculation itself.

The results from our analysis of the maximum number of particles per clump in section 7.3.1, demonstrate that calculation rates remain significantly higher even when calculations for only a few particles are performed. The cost of reading the node data into the cache blocked array and then re-reading it multiple times is both small and can be amortized effectively over the calculations of only a few particles. Cache blocking will therefore remain effective even when only a small fraction of the particles in a clump require updates, as will often be the case when an individual time scheme is used. Speed differences due to page size effects will become somewhat more pronounced however because the ratio of time spent in the traversal itself, compared to the multipole summation, becomes less strongly weighted in favor of the summation. In the extreme case, when only a single particle requires a calculation, we expect the scaling to be similar to the curves shown for the level four optimization in figure 8. Since most of the time in any calculation is spent evolving a much larger fraction of the particles than this, the benefits of the cache blocking optimization will remain substantial.

7.3.3. *Performance of the SPH calculation and additional benefits of particle reordering*

In SPH simulations, the cost of the hydrodynamic calculations is second only to the cost of the gravity calculation and therefore also benefits from parallelization and optimization. Here we examine the speed of a single calculation of all hydrodynamic quantities using the initial and evolved versions of the SPH test problem, and the improvements that can be obtained by the particle reordering optimization discussed in section 3.5. While we expect that, overall, similar speedups in the SPH calculations will be derived from the various memory layout optimizations described in section 7.3.2, we have not tested these specifically. Instead, we examine only one additional optimization not tested before—reordering the particle data themselves. We also limit our tests to only the 64kB and 16MB page size variants.

In figure 9, we show the speed of a single calculation of the SPH quantities for both the initial and evolved SPH test problem, before and after reordering the particle data according to the second reordering variant in section 3.5. Overall scaling of the fully optimized ver-

sions are excellent, though slightly below those of the gravity calculation, with speedups of nearly a factor between 90 and 100 out of a theoretical maximum of 120. The raw speeds of the SPH calculations, at ~ 13900 particles per second per processor for the initial condition and ~ 12900 for the evolved condition, are just under twice those of gravity (figure 8). The raw and scaled performance of the evolved condition falls below that of the initial condition by $\sim 10\%$, but we are encouraged that performance does not degrade more noticeably in either case, a possibility not otherwise neglectable if the particle distribution had played an important role in the scaling.

The left hand panels of figure 9 show performance prior to the reordering. As for the gravity calculation, the rates are highly sensitive to page size, with a performance enhancement of a factor ~ 2.5 between 64kB and 16MB pages for both initial and evolved conditions. Further performance enhancements of 10% occur for the large page variants when the particle data are reordered, over and above that obtained from the reordering already done in the tree itself, and enhancements of 20% or more were common in tests performed on other architectures (not shown here). While scaled performance using small pages is good, raw performance falls significantly below the large page variants, even at high processor counts where performance of the large page variants has saturated. Reordering the particle data removes all signs of saturation and both large and small page variants run with nearly equal performance, demonstrating the effectiveness of the reordering at insulating the simulation from limitations of the hardware.

7.3.4. *Performance of the tree build and revision*

Constructing and revising the tree together make up the third most costly component of particle simulations with VINE. In figure 10, we show the speed of a complete tree rebuild for the N -body test problem, before and after reordering the particle data in memory, according to the discussion in section 3.5. In figure 11 we show the speed of a tree revision.

On a single processor, the tree build proceeds at rate equivalent to 5×10^4 particles per second with all optimizations, while the revision proceeds at a rate equivalent to 7.3×10^5 particles per second. These rates correspond to ~ 7 and ~ 100 times faster than one gravitational force calculation for the same particle distribution. As for the gravity and SPH calculations, parallel scaling is better with small hardware pages, and raw speed is better with large pages. Before data reordering, the large page (16MB) version runs a factor ~ 3 faster than with small (64kB) pages. Also as with gravity and SPH, reordering the particle data improves the raw performance of the tree build, in this case by a factor of two, due both to better cache and TLB reuse. After reordering, the speed is substantially less sensitive to page size, indicating that most of the benefits of large pages can be obtained even on architectures where they are unavailable, simply by reordering the particle data in memory.

While both build and revision clearly benefit from parallel operation, neither yields the linear scaling with processor count seen for the gravity and SPH calculations. Instead, their scaled parallel speedups saturate at factor of ~ 11 and ~ 16 , respectively, on 120 processors.

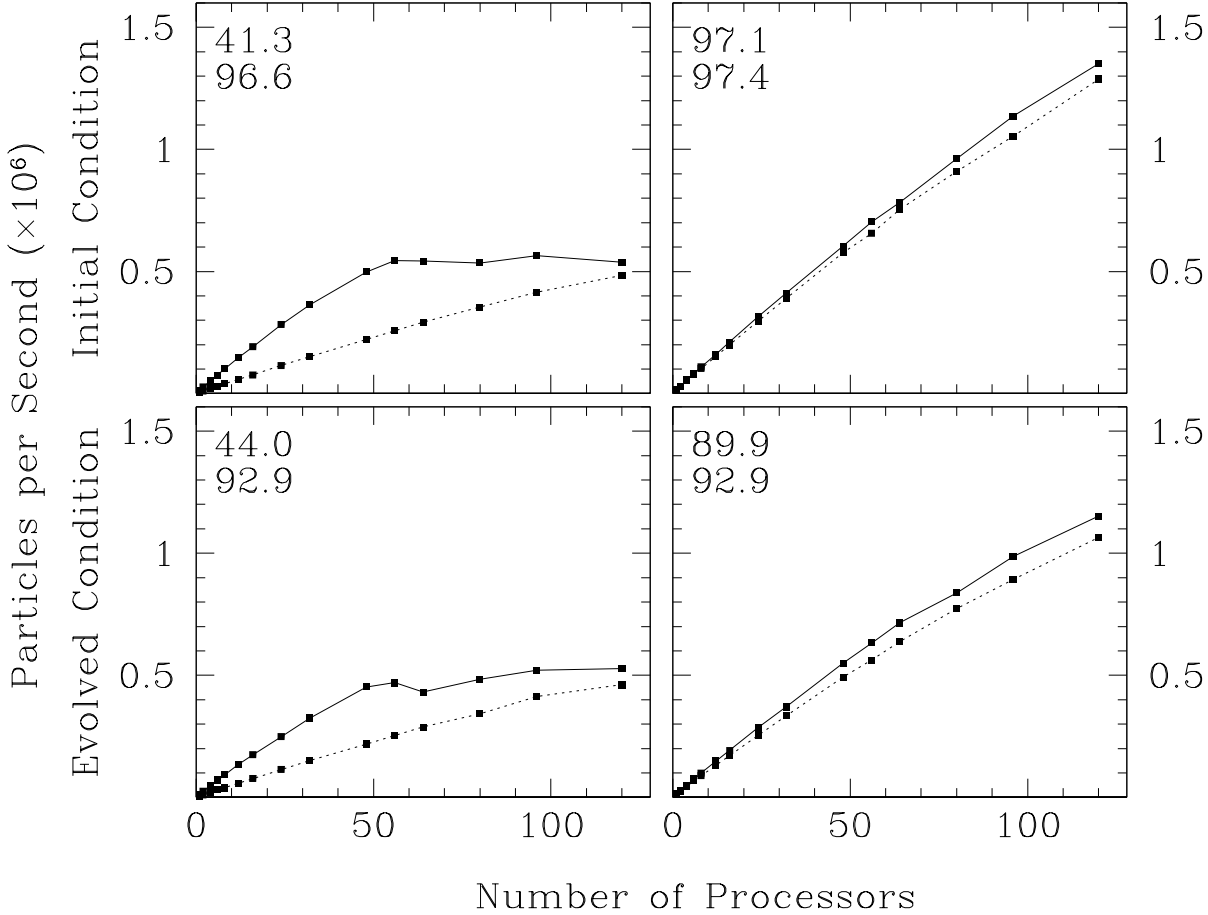


FIG. 9.— Calculation rate for a single SPH calculation for the SPH test problem initial condition (top panels) and the evolved condition (bottom panels), each before (left panels) and after (right panels) reordering the particles locations in memory. The solid lines indicate results obtained with 16MB page sizes, and the dotted lines results obtained with 64kB page sizes. Numbers in the upper left corner of each panel indicate the scaled parallel speedup for the realizations with 16MB (top) and 64k (bottom) page sizes plotted in the panel, respectively, out of a maximum of 120 for linear speedup.

Also, though not shown here, we note that highly clustered particle configurations can degrade both the absolute performance of the build and its scalability to some extent. In the case of the SPH evolved test problem, in which mass density varied by several orders of magnitude in comparatively ‘smooth’ regions and up to $\sim 10^{12}$ in regions where stars had begun to form, we measured performance loss to be some 20-40% (depending strongly on the architecture tested) over the initial condition. Although we cannot be satisfied by either the saturation or the sensitivity to particle configuration, we are at least comforted by the fact that performance does not actually decrease, a very real possibility for parallel codes when communication costs become significant.

Despite similar appearances, the factors limiting parallelism in each case are not identical. For large processor counts, the ultimate limiting factor affecting both routines is that latency between a given processor and the data on which it operates is a function of data placement. It will be both different for each processor and intrinsic to the NUMA fabric of the system itself, so that even when ostensibly equal amounts of work are given to each processor, load imbalance develops due to differences between the times required to load and store data to and

from memory. We believe that data placement issues such as these are also the source of the scatter in scaling seen especially in figure 11 for processor counts > 24 , as data distribution among the processors and memory becomes more dispersed and placements with some processor counts are more beneficial than others. Although we have performed no systematic study to verify this hypothesis, in a few, exploratory tests we have noted significant timing differences between identical runs performed on different sets of processors spread across different nodes in the NUMA fabric. Such differences lend support to our conclusion.

Tree construction suffers from two additional limitations which, together with NUMA, contribute roughly equal proportions to the overall performance degradation. First, we estimate that $\sim 1 - 2\%$ of the tree build cost remains serialized due to unavoidable dependencies between different units of work. Second, as tree construction proceeds to higher levels, fewer and fewer nodes remain to be shared among processors so that they become progressively more starved for work, generating relatively large load imbalances, synchronization and communication costs. These costs become especially significant for highly inhomogeneous particle distributions, as

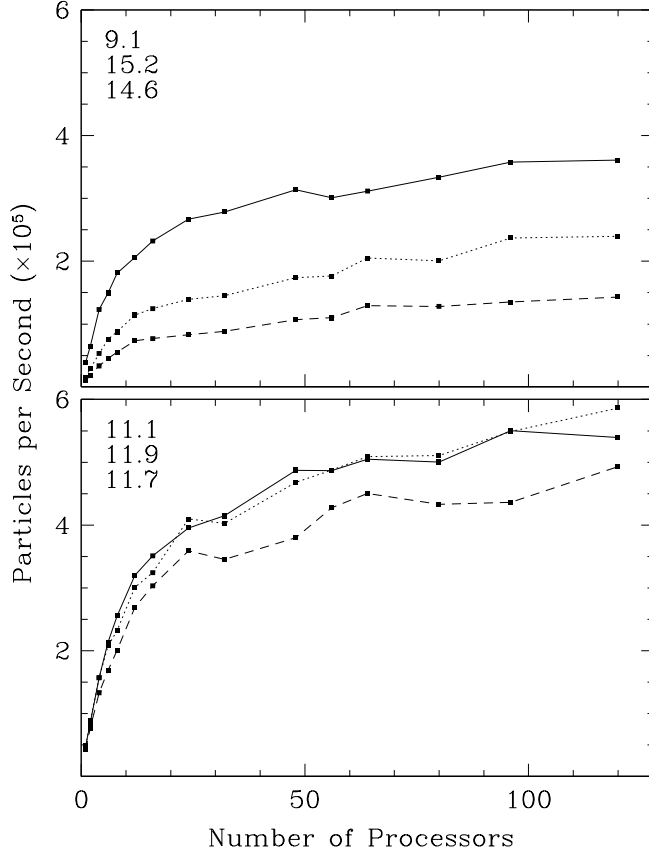


FIG. 10.— The speed of a single tree rebuild, before (top panel) and after (bottom panel) reordering the particle data in memory, as a function of number of processors. The three curves correspond to the build done with 16MB pages (solid), 1MB pages (dotted) and 64kB pages (dashed). Top to bottom, the numbers in the upper left refer to the scaled parallel speedup for the 16MB, 1MB and 64kB page sizes, respectively, out of a maximum of 120 for linear speedup.

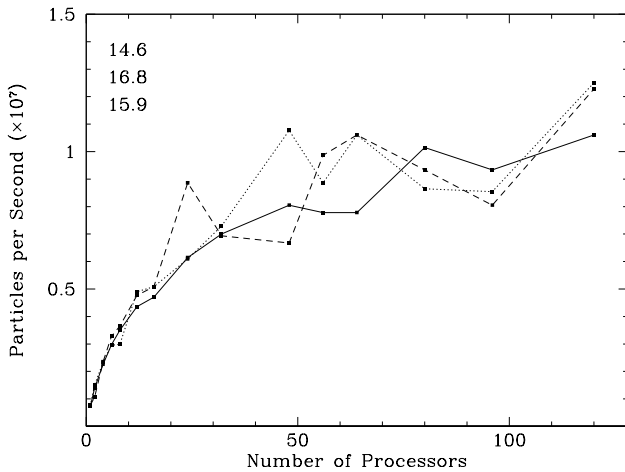


FIG. 11.— The speed of a single tree revision.

in the case of the evolved SPH test problem, because fewer nodes are created per level, especially near the root. We believe that although a few improvements could be made to mitigate the effects of these limitations somewhat, they will never be entirely removable. Section 7.3.6

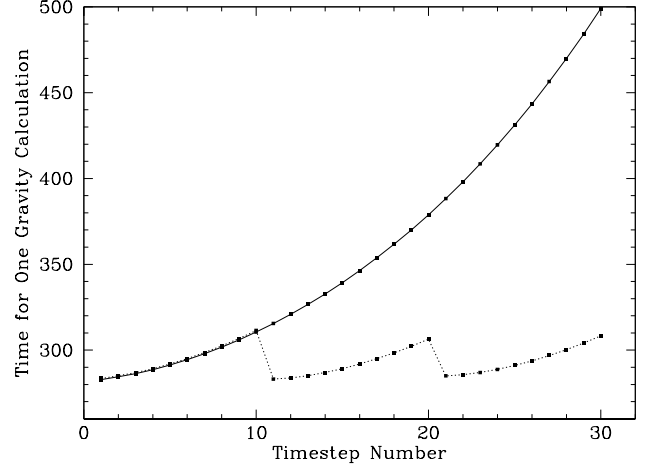


FIG. 12.— The time required for a series of time steps of the N -body test problem, for which the gravitational force calculation entirely dominates the total. The solid curve indicates the times required for each of 30 time steps with no tree rebuilds, while the dotted curve indicates the times required with a complete tree build spaced every ten time steps.

demonstrates however, that their effects will become less and less important for larger simulations because a comparatively smaller fraction of the build time is spent at the highest levels of the tree, where work starvation is most severe.

7.3.5. Frequency of Tree Rebuilds

Combining the information in figures 7, 10 and 11, we calculate that a tree build or revision will be, respectively, factors of seven and 100 faster than a single gravity calculation on one processor, and so will contribute little to the total simulation time in serial and small scale parallel operation. Their contributions will become more significant in highly parallel simulations and when only a fraction of the particles require force updates, as when individual time steps are used.

As noted in section 3.7, the tree does not need to be rebuilt after every time step but can instead be used for several in succession with only an update of the node data to the current time, saving computing resources better spent directly evolving the particles. Of course, rebuilds must still occur occasionally because particles move with respect to one another, causing their parent nodes to become larger and larger. Larger nodes affect the speed of both the SPH and gravity calculations because more and more nodes must be examined for acceptability, and more and more nodes must be included in the multipole summations. In this section, we attempt to determine the optimal frequency of tree rebuilds.

When the code is used in global time step mode, the frequency for rebuilds can be determined easily based on the time required to update the system immediately after a tree build as compared to the time required after some number of time steps have elapsed. We illustrate this slowdown in figure 12, where the time for successive force calculations is plotted as a function of the number of time steps since a complete rebuild, during the evolution of the N -body test problem with global time steps. Over the course of 30 time steps, the time required increases ever more rapidly as particles and nodes become more and more separated from their initial nearest neighbor

status. Enforcing a tree rebuild every ten time steps returns the calculation times again to their original high efficiency. Since a full reconstruction of the tree requires ~ 30 s on 8 processors of the Origin 3000 on which this test was performed, and the time for one update increases by an approximately equal amount over 10 time steps, a reasonable spacing between rebuilds is once per $\sim 5 - 10$ time steps.

The question of how often to rebuild the tree is not trivial when the code is used with individual time steps because it is difficult to determine—on a particle by particle basis—when a calculation requires sufficiently more time that the cost of a tree rebuild would be less than that of an update. It would also be beneficial to have some process by which the user would not be required to tune the rebuild frequency for a given problem in a global time step calculation, but rather to have a single parameter by which the rebuild/revise decision could be made automatically. Since force calculations using the tree will be sensitive to the physical size of the nodes in the tree through the node opening criteria, one such parameter can be defined using the increasing physical size of clumps, as defined in equation 6, as a proxy for the increasing size of all of the tree nodes. This value is required for other calculations and will therefore allow the code to make a decision to rebuild the tree at essentially no additional cost.

In figure 13, we show the clump size distribution, relative to their original sizes, after a number of time steps have elapsed since the rebuild, for the same calculation shown in figure 12. After 10 time steps have elapsed, some clumps have expanded to as much as twice their original radius, after 20 steps, well over three times their original radius, and after 30 steps, over four times their original radius. Decreases in size also develop, in this problem to about 80% of the original size. The ratios are near log-linear in distribution, so that specifying a given maximum ratio will be an effective proxy for specifying the full distribution. Noting from figure 12 that an increase in computation time per time step of 30 seconds (about that of one tree build), corresponds to a maximum increase in clump radius of a factor of two, we can conclude that triggering a rebuild when the size of any clump changes its radius by a factor of two, we will be able to automatically retain most efficient calculations of the forces. Experiments on several particle morphologies indicate that this factor is comparatively insensitive to particle distribution, though still other distributions may prove more so, and may require another factor be used. Users may change its value through a setting in a text input file, read in by the code at run time.

7.3.6. Performance on problems of different size

So far, we have demonstrated the parallel scalability of the code on problems of moderate size, at times when all particles require force calculations. In practice of course, the code will be used differently in two important respects. Simulations will be run with different sizes than we consider and they will be run using an individual time step scheme, so that only a small fraction of the total number of particles require updates at any given time. Due to the unpredictability of load balance and work distribution among time step bins, it will not be possible to address the latter concern with any general-

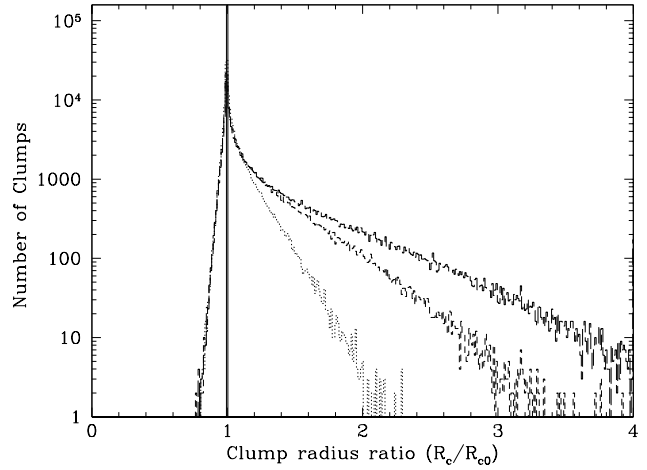


FIG. 13.— A histogram of the ratios of the physical radius of a clump several time steps after the tree build, to the value immediately after the build. The solid curve shows the ratios at time step zero (i.e. all ratios unity), while the dotted, dashed and long dashed curves show the distribution after 10, 20 and 30 time steps, respectively.

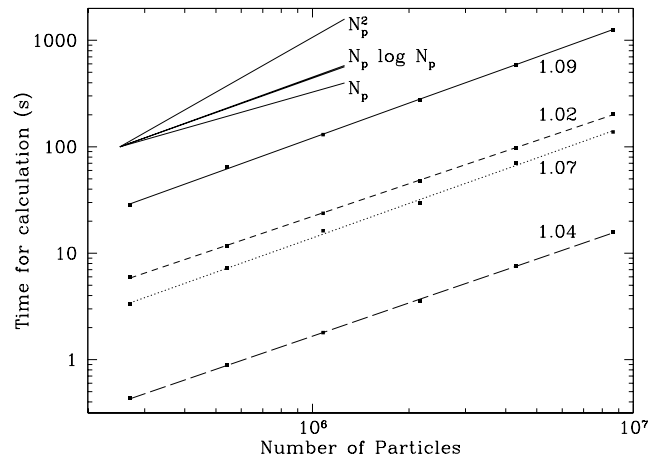


FIG. 14.— Time required to perform one gravity calculation (solid), one SPH calculation (dotted), one tree build (dashed) or tree revision (long dashed), for an identical initial condition realized with six different particle numbers. Points represent actual timings, while the lines represent a linear fits to the logarithms of each coordinate. The scaling (i.e. the linear term in each fit) is indicated adjacent to each. Lines in the upper left corner represent scalings proportional to N_p^2 , $N_p \log N_p$, $N_p^{1.09}$ and N_p , as indicated. Only three lines are visible because the curves for the $N_p \log N_p$ and $N_p^{1.09}$ proportionalities over lie each other.

ity. We can still gain some insight into the scalability by looking at identical problems of different size however. In this section, we examine the sensitivity of the overall performance and the parallel scaling of the code using six realizations of the galaxy merger test problem at different resolution, and which include both SPH and N -body particles, as defined in table 2.

Figure 14 shows the time required to perform one complete calculation of each of the major components of the code on one processor of the Origin 3000. As expected from theoretical considerations of the tree algorithm itself, proportionalities for the gravity and SPH calculations are steepest, with the slope for gravity corresponding exactly to the value expected over this range for a

curve with $t_{\text{grav}} \propto N_p \log N_p$. The proportionality for the SPH calculations is lower because, while the tree traversals required for the neighbor searches scale with $N_p \log N_p$, calculations with the resulting lists of neighbors scale only proportional to N_p . Both the tree build and revision follow still shallower proportionalities, so that as problem size increases, their costs decrease relative to gravity and SPH. As seen for the N -body and SPH tests above, the absolute cost of the gravity calculation is higher than any other part of the code, but because only $\sim 14\%$ of the total particles in the six Merger tests are SPH particles, the tree build replaces SPH as the second most costly calculation, with the tree revision an additional order of magnitude cheaper than either. The excellent scaling of each component over a factor of 30 in size indicate that simulations of any size with VINE will be possible with both predictable and affordable cost.

Figure 15 shows the scaled parallel efficiencies of each code component for each of the realizations at different resolution. Even at comparatively low resolution, the efficiency of the gravity calculation is excellent. Only small deviations from linear scaling are visible for the low resolution (270000 particles) run up to ~ 32 processors. Above that count the speedup continues to increase to the limits of the machine, but no longer follows a perfect linear relationship, ending in a $\times 50$ improvement on 120 processors. Each of the higher resolution variants follows the same pattern, with the performance knee shifted to progressively higher processor counts. For the highest resolution version, a small deviation from linear performance becomes visible only above ~ 80 processors, dropping to 110 at the 120 processor maximum for the machine.

The curves for the SPH calculations also show very good scaling up to ~ 32 processors though, as for the SPH test problems above, below that achieved in the gravity calculation. Above 32 processors however, rather than continuing to improve up to the limits of the machine, all of the curves instead turn over and saturate near a factor ~ 50 . Also in contrast to the gravity calculation, relatively little differentiation between the scalings at different resolutions is visible. The plateau appears to be due in part to the fact that only $\sim 15\%$ of the total number of particles are SPH particles and to the small total number of SPH particles in these simulations. Both characteristics increase the likelihood for load imbalance at high processor counts. The scaling limits are important to quantify because, in some respects, the fact that SPH particles are distributed irregularly throughout the tree mimics the behavior of the code when simulations using individual time steps for each particle are run, and active particles are distributed irregularly throughout the tree.

For both construction and revision scaling is good up to $\sim 5 - 8$ processors at all resolutions, but saturates at higher levels of parallelism, as we found in our tests in section 7.3.4. Above eight processors, the curves for different resolutions become differentiated from one another. The curves for the tree build are relatively smooth functions of processor count, and are well distinguished from both their higher and lower resolution cousins. Performance of the lowest resolution variant does not increase beyond a factor $\sim 3 - 4$ speedup, but the saturation level increases in progressively higher resolution vari-

ants, eventually to a speedup of ~ 12 for the highest resolution case. For still higher resolution simulations, we expect this trend to continue because a relatively smaller fraction of the total will be spent associating nodes near the root of the tree, where the total number of unassociated nodes is small and parallelism ineffective.

The revision scalings display much more irregular patterns. For our highest resolution variant, scaling increases steeply to ~ 16 processors, then more shallowly to a factor ~ 20 at the high end limit of our study. Lower resolution variants fall off at progressively fewer processors, but the curves sometimes intersect each other and, in some cases, actually decrease slightly before increasing again. We attribute the irregularity to the fact that the revision requires only a very small amount of total time (typically much less than a second, especially for the lower resolution tests), so that sensitivities to systematic effects such as data placement in the NUMA hierarchy play a proportionately larger role. Attempts to repeat a subset of the timings appear to confirm this hypothesis, as timings for different runs could differ by as much as several tens of percent in otherwise identical runs, done at different times on different distributions of processors.

Overall, these tests demonstrate that the code's efficiency scales very well both to very large and to very small problem sizes. For small problems, performance may no longer increase linearly beyond $\sim 30 - 50$ processors, but in no case do we find the overall scaling to decrease with additional processors, even for very low resolution simulations where even small load imbalance and interprocessor communication can become significant. This is important for simulations utilizing individual time steps for each particle because only a fraction of the total complement of particles will require updated force calculations at any given time.

7.4. Performance on other architectures

The Origin 3000 architecture on which the tests in sections 7.2 and 7.3 were performed is only one of a number of shared memory systems on which VINE can be run. It is also, at this writing, a retired architecture for which no succeeding system exists using the same processor, though the Altix machine plays a similar role using Intel Itanium 2 processors and a somewhat similar interconnect fabric to connect processors and memory. Other large scale, shared memory parallel systems are commercially available from IBM, Sun and HP. Desktop machines with multiple processors have also become common and we can only expect this trend to continue to larger scales in the future as machines with more processors, and processors with more cores per chip, become commonplace.

In this section we compare the performance of the code on a several hardware architectures and compilers, referenced in table 3. Because many of these machines are from different computer 'generations', a direct comparison of one processor type against another will not be particularly meaningful as an indicator of some overall best architecture or processor, and readers are cautioned to be mindful of this fact in making such comparisons. On the other hand, correlated with user experience of speedups expected between one generation and the next within a single processor family, some inferences may be justified. In any case, the comparisons will be useful as

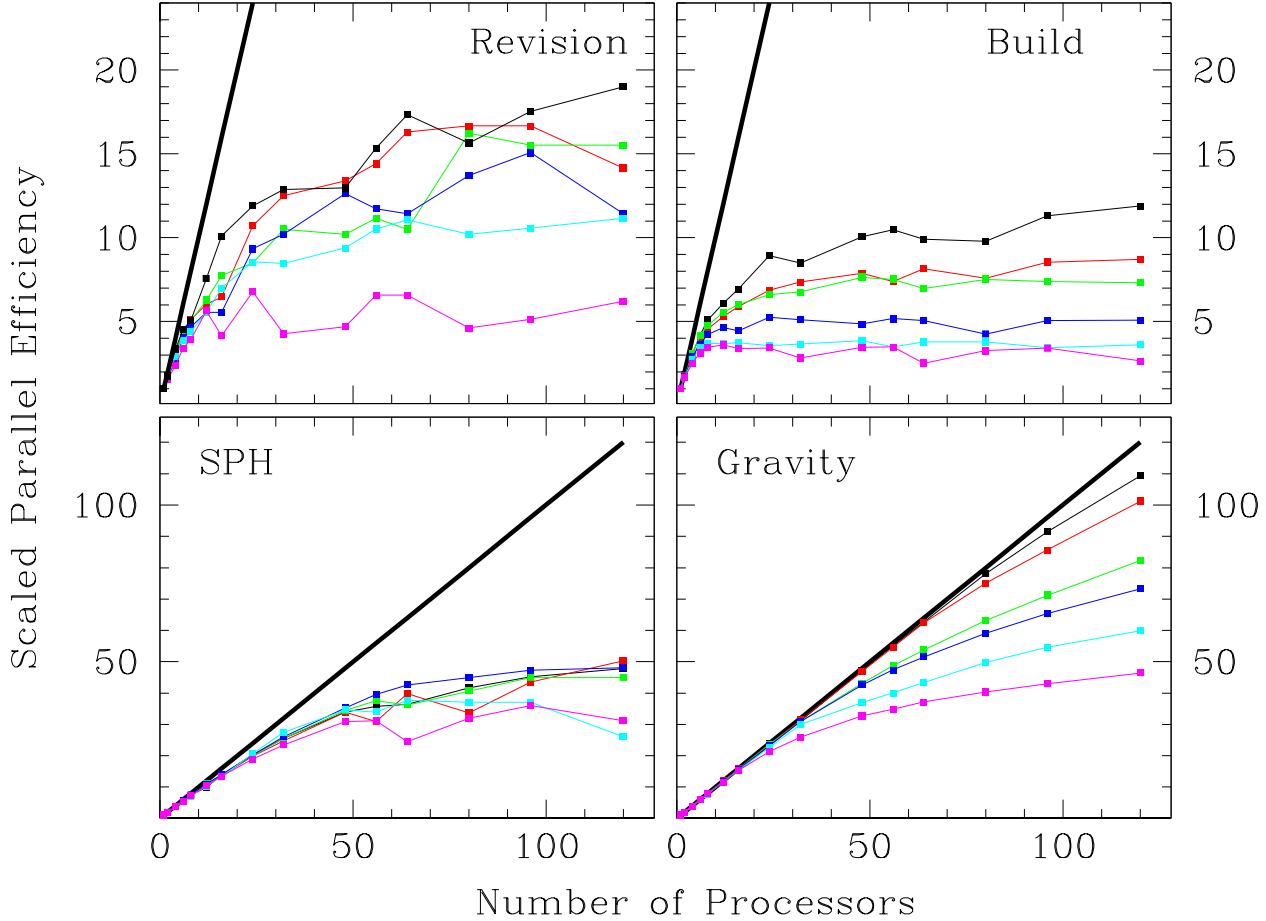


FIG. 15.— Parallel scaling of the same calculations shown in figure 14 for realizations at each resolution. The heavy solid line in each panel delimits perfect linear scaling. In order from high to low resolution, each curve corresponds to the color black, red, green dark blue, light blue and magenta.

a relative indicator of how the code performs on exactly the same problem across a wide variety of machines, possibly assisting heavy users of the code in the selection of one machine over another to which to commit resources.

7.4.1. Serial performance

In figure 16, we show calculations rates for single processor tests, on five different processors for each major component of the code. For the gravity calculation, the clear ‘winner’ is the Intel Itanium 2 processor, with calculation rates of a factor 50% faster than its nearest competitor, the Power 5. Its performance is also a factor ~ 5.5 faster than the R12000 processor on which the detailed performance analyses above were made. For all other components, performance of the AMD Opteron is highest, at a factor ~ 1.4 faster than its nearest competitor (Itanium) for SPH and ~ 4.1 times faster than the R12000. Comparable figures apply to the tree build and revision as well.

A number of features of figure 16 are of interest. First, the superior performance of the Opteron is, to some extent, to be expected since it is more recently made than any other processor in our sample. The fact that its performance on the gravity calculation falls between that of the two Power processors is a significant drawback to its performance overall because of its large total cost

for most simulations of interest in astrophysical contexts. Also, although its serial performance is very good, no machines are currently commercially available which exploit the high performance in large scale shared memory configurations, so the higher serial performance may only be useful for comparatively small simulations, where highly parallel operation is not required.

The raw performance differences between the Power 4 and Power 5 processors are remarkably small, corresponding roughly to differences in clock speeds between the two processors. In comparison, differences between their performance on the well known SPEC CPU2000⁸ benchmark suite would lead one to believe that improvements nearer a factor two or more were to be expected. Also, their performance is disappointing on the SPH and tree calculations relative to the much older R12000 processor, at factors of only $\times 2$ and $\times 2.5$ faster, respectively, though the gravity calculations do somewhat better at factors of $\times 2.5$ and $\times 3.6$.

When we compare the rates derived from the merger test simulations done in Vine1 with those shown in figure 16, we notice an important discrepancy. The rates for the merger test in Vine1, of ~ 70 kparticles/s for 8 Itanium 2 processors, are far lower than would be expected

⁸ <http://www.spec.org>

TABLE 3
COMPUTER ARCHITECTURES TESTED

Machine	CPU type	Compiler	Identifier
SGI Origin 3800	128× R12000 (400MHz)	Mipspro 7.4.2	1
IBM p690	32× Power 4 (1.3GHz)	xl f 9.1	2
AMD Opteron	2× Opteron (2.4GHz)	Pathscale 2.3.1	3
IBM p575	16× Power 5 (1.65GHz)	xl f 9.1	4
SGI Altix 350	56× Itanium 2 (1.5GHz)	Intel 9.1.33	5
SGI Altix 350	(GRAPE-6A related tests)	Intel 10.0.25	

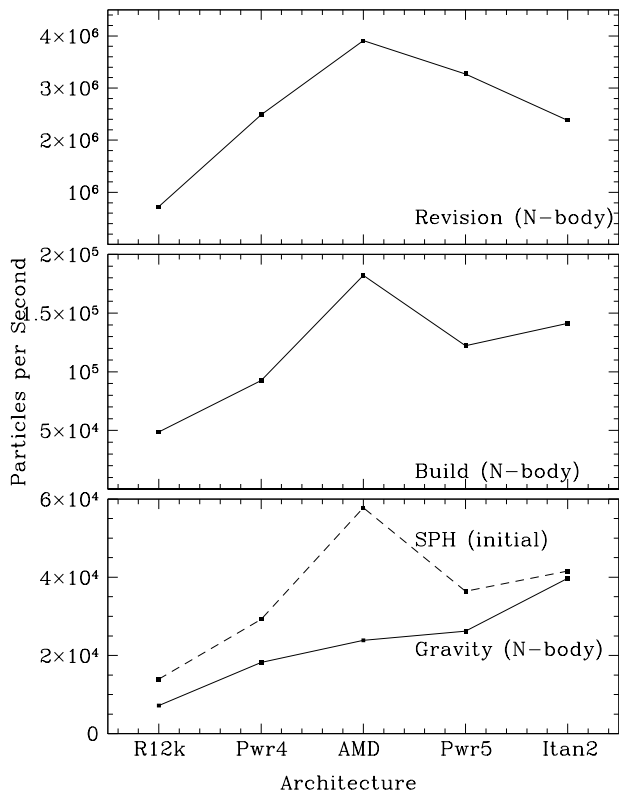


FIG. 16.— Calculation rates for the gravity, tree build and revision calculations on the N -body test problem, and the SPH initial condition, running on a single processor of the specified type. Each plot is ordered from left to right according to increasing performance of the gravity calculation. The SPH evolved condition (not shown) follows the same pattern as does the initial condition, at an overall speed $\sim 10\%$ slower than the initial condition.

from a simple extrapolation of the ~ 40 kparticles/s for one Itanium 2 processor shown here. The rate differences appear to be due to two effects. First, the mass distributions are not the same. While the N -body test problem is spherically symmetric system with $r^{-1/4}$ density profile, the merger simulation consists of two more or less separated galaxies at various times during their merger evolution. Second, and more importantly, the merger simulation consists of several types of particles, each with their own masses and gravitational softening lengths. When larger softening lengths are used, the node size of all parent nodes increases proportionally (see equations 5 and 6), and will therefore result in many additional node examinations during the tree traversal, and the addition of many additional nodes to the interaction lists themselves. The rate differences between these different con-

figurations do not affect the conclusions in Vine1, that VINE is $\sim 4\times$ faster than Gadget-2 however, since the speed comparisons for that test were done using exactly the same particle configurations for each code.

As is to be expected given its much greater age relative to the others, the performance of the R12000 processor falls substantially behind that of all the other processors in our sample. This is important because the performance characteristics of VINE discussed above will be better on architectures commonly available today in proportion to the speedups seen in this plot. It is of some interest that the magnitudes of the speed increases are somewhat smaller than might be expected from a naive application of Moore's Law.⁹ Some deviations from the expected speedups may be due simply to hardware features that VINE exploits more fully on one processor family rather than another, or on one workload rather than another. The fact that some of VINE's calculations speed up more than others across different processor types illustrates clearly that no single architecture dominates all aspects of the calculations required for astrophysical simulations.

7.4.2. Parallel scaling

Figure 17 shows scaled parallel efficiencies for the four major components of the code on several architectures. The parallel scaling of the gravity calculation is near linear with processor count for all architectures tested, up to the limit imposed by the size of the machine itself. Of the four architectures, performance on the Altix fared comparatively least well, falling to 'only' $\times 29.5$ and $\times 44$ speedups out of 32 and 48 processors on the two largest tests, respectively. In comparison, the Origin 3000 and Power 4 based p690 machines gave speedups of 31.5 and 31.1, respectively, when run on 32 processors.

The scaling of the SPH calculations is also excellent, with near linear speedup in the SPH calculations on three of the architectures tested, to the limits of each machine. Performance on the Altix is an exception however, deviating from linear speedup near $\sim 8 - 16$ processors and eventually dropping to a comparatively poor factor $\times 22$ speedup on 48 processors. Much larger disparities, among all of the systems in our test, are present in the tree build and revision procedures. The Power 4 based p690 realizes the best performance on both, reaching speedups of ~ 9 and ~ 16 on 16 or 32 processors, respectively, while the other three realized speedups between $\times 5$ and $\times 10$, even when run on more processors. Paral-

⁹ Although by its actual definition, Moore's Law refers to a time scale for doubling the component density per processor, we apply it here in its commonly misused form as a speed doubling every 18-24 months.

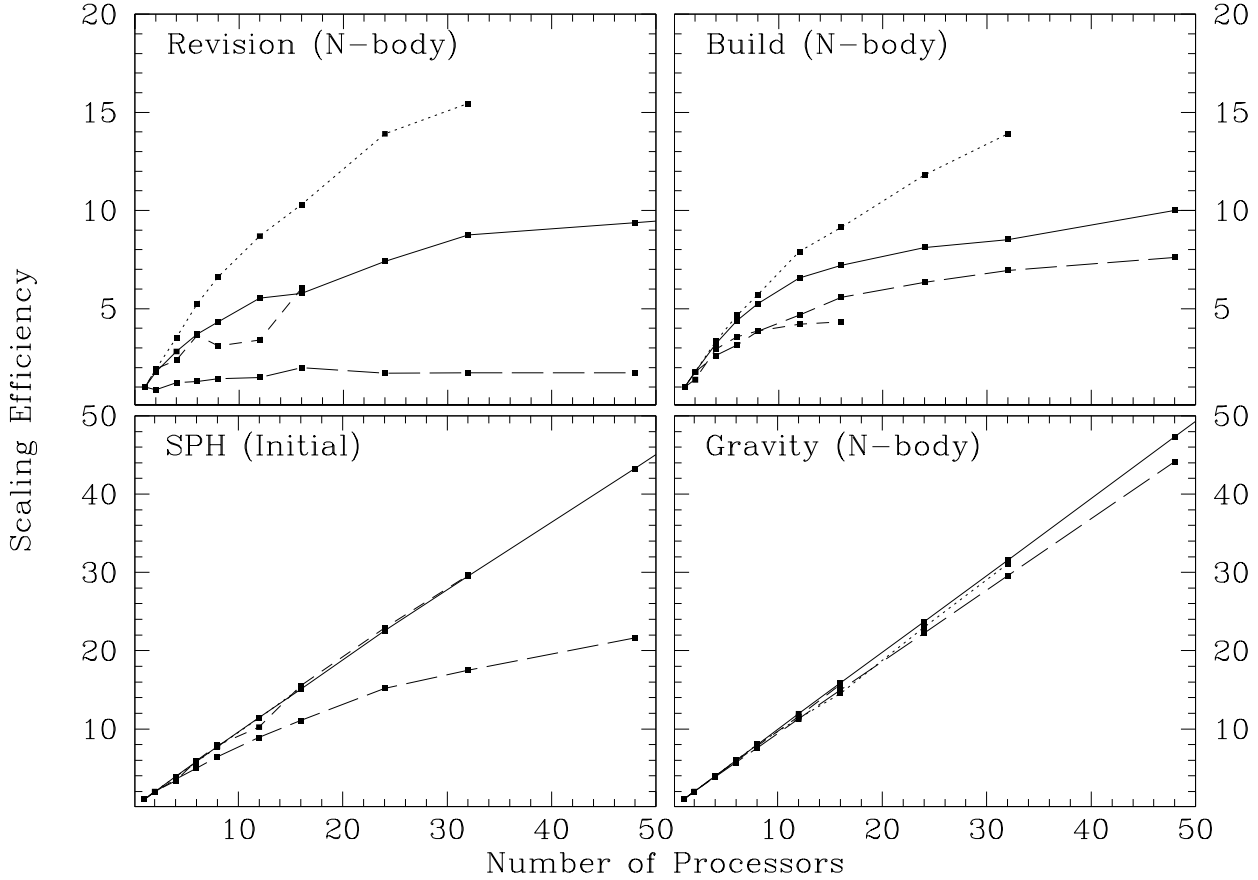


FIG. 17.— Parallel scaling of the major components of the code, for a number of different architectures. Tests of the SPH evolved condition mirrored the results of the initial condition and are neglected here. The curves correspond respectively to the SGI Origin 3000 (solid), IBM p690 (dotted), IBM p575 (short dashed) and SGI Altix (long dashed). Curves for each architecture extend different distances along the x axis depending on the size of the machine on which the tests were made.

lel scaling of the tree revision on the Altix machine saturated at an even lower plateau of a factor ~ 2 speedup, no matter how many processors were used.

Of some interest are the differences in scaling between the Power 4 and Power 5 based machines and, to a lesser extent, also between the Origin and Altix machines, due to the architectural similarities between each pair. In fact, limited correlation can be seen in the performance between the two pairs, even though the code and data are identical. We have not attempted to explore the origin of the performance disparities, but nevertheless can make some conjectures, based on the kinds of calculations made in each of the different procedures. Specifically, that the differences are due to the complicated interactions between the processors and the memory they use. Procedures with a small memory footprint, even if they consume huge amounts of processing time as do the gravity and SPH calculations, scale consistently well. Procedures that cycle through large volumes of memory but perform few calculations, as do the tree build and revision, scale less well and inconsistently across architectures.

It is of some disappointment that the Altix architecture, theoretically scalable to higher processor counts than any other, does not perform as well as the others on the latter workload, since a non-negligible fraction of VINE's total workload includes such operations.

As an example of the consequences that will result in practice, we point out the scaling behavior of the SPH calculation. Examination of its various components on Altix show that the density and hydrodynamic force calculations, which together account for $\sim 98\%$ of the total time on one processor, and which do a large amount of work using a small volume of memory accessed repeatedly, do in fact scale linearly with processor count. On the other hand, while other components, such as the equation of state calculations or the smoothing length derivative which each cycle through a large volume of memory performing only a few operations per particle, require only $\sim 2\%$ of the total time on one processor, their parallel performance is quite poor, in some cases actually decreasing with processor count rather than increasing. Specifically for the Origin/Altix architecture pair, we may ask the question ‘can we attribute the scaling differences between our tests to differences in memory distribution mechanisms in IRIX and Linux?’

The comparisons in this section neglect several architectures and processors entirely, largely because we were unable to secure time on such machines, and because of simple limitations in the amount of effort required to perform the desired tests. Of the machines in our comparison, the best overall serial performance for users of VINE will be obtained on machines using Itanium 2 processors, especially for simulations of purely N -body systems. Due

to their excellent performance in all other components, AMD Opteron processors may also provide comparable performance in simulations with both self gravity and hydrodynamics. No tests of the parallel scalability of machines using the AMD processors were performed because at the time these tests were performed, highly scalable, shared memory machines using AMD processors were not yet commonly available¹⁰. Best overall performance will be achieved when using machines based on Power processors.

7.4.3. *Effect of large pages on other architectures, and difficulties associated with their use*

In sections 7.3.2, we demonstrated the large sensitivity of the code's speed to the hardware page size on the Origin 3000 architecture using MIPS R12000 processors. In general, we cannot expect the same sensitivity across all processor families because some include circuits to calculate TLB entries directly, while others, like the R12000, compute new entries in software by the operating system. In this section, we explore the sensitivity of the code to page size on the Power 5 processor, in order to demonstrate that the sensitivity is not specific to a single processor family, and to demonstrate that the performance optimizations we have made also provide benefits on other architectures as well. For reasons we discuss below however, we point out to readers that direct speed comparisons with results in other sections should not be made, because the tests were run at a different time and different settings were used to produce the results.

Figure 18 shows gravitational force calculation rates obtained from simulations run using Power 5 processors, as a function of processor count. As with MIPS, performance of the non-cache blocked version of the code is greatly enhanced when large pages are available and are used, in this case by a factor 1.65. The differences decrease to only $\sim 5\%$ in the cache blocked versions, where we expect the effect should be minimized. We conclude that the sensitivity of the code speed to hardware page size is not specific to any one processor family, but reflects a general property of the code itself. The magnitude of the sensitivity will vary somewhat from family to family, depending on the implementation of the TLB refill process itself. The benefits seen on the Origin architecture may be particularly large due to this fact, because MIPS processors require software intervention for their TLB refills.

In contrast to the R12000 processor, the difference between non cache blocked and cache blocked versions with large pages is also substantial. Cache blocking improved performance by a factor ~ 1.6 on the Power 5, compared to only $\sim 17\%$ on the R12000. As we expect, both processors improve by more substantial margins when small pages are used, so that the both the large and small page variants obtain similar performance. We conclude that other sources of memory latency are much more significant on the Power architecture than on the Origin 3000, though we have not attempted to isolate the exact origin more fully.

Given our conclusions, it is important to note as well that the ease and flexibility of actually using large pages

can vary widely between architectures, and even between operating systems using the same architecture (e.g. Linux or AIX on Power processors). On the Origin 3000 architecture, where the sensitivity to page size was initially seen as the code was developed, use of large pages was straightforward and we were regularly able to test the effects of various alternative optimizations on the code speed. Even on this system however, consistently obtaining the same page distribution from run to run (when the desired page size is unavailable, the operating system falls back to other page sizes) was frequently difficult or impossible, yielding benchmark data contaminated by one or more data with a mixed distribution of page sizes. To minimize such disruptions in timings discussed in this work, we monitored the page sizes used in the run with system tools designed for the purpose, and reran tests where contamination was unmistakable.

On other architectures, such as the IBM Power series for example, special coordination with system administrators was required to make any tests at all, because of instabilities introduced into the machine and operating system by the use of large pages. Although we were able to perform the series of preliminary tests illustrated in figure 18, large page use in production was disabled on the machines due to the resulting unacceptably severe instabilities in the operating system that resulted from their use. For this reason, later performance tests using identical code settings as were used in figures 7 and 8 were not possible. On still other systems, large pages can only be utilized if the code is rewritten to take advantage of special memory allocation calls, such as those implemented in Linux through the 'hugetlbfs' infrastructure. We did not pursue this option, due to its cost both in programming time and to portability.

Fortunately for users of VINE both on the Origin architecture and on others where large page use is more restricted, the optimizations described in this paper demonstrate that a properly implemented code may realize many of the benefits of large pages, even when only small pages are available on the machine where the code is run. Performance will still be less than optimal when the code is used in its individual time step mode however, because the effectiveness of the cache blocking optimization will be reduced.

7.5. *Performance of the GRAPE+tree option in VINE*

As we continued to develop VINE, more advanced versions of GRAPE hardware became available and modules implementing interfaces to them were added to VINE's code base. In this section, we discuss the performance of the combined GRAPE+tree option in VINE, in which we use tree traversals to reduce the total number of nodes needed to determine the force on a given particle, but send those nodes to a GRAPE co-processor board for calculation rather than using the host processor itself.

We use several variants of our N -body test problem, each at different resolution, and each using the optimal maximum bunch population for that problem size as discussed in section 7.3.1. In addition, we test the speed with a 2^{21} particle homogeneous sphere configuration, which we have configured to have identical characteristics to the same configuration discussed in Fukushima et al. (2005, hereafter FMK05). The system of units is chosen such that $M = G = 1 = -4E$ where M is the total

¹⁰ More recently, machines incorporating dual and quad core processors in multi-socket motherboards have become commonly available, though we have not yet made tests on these machines

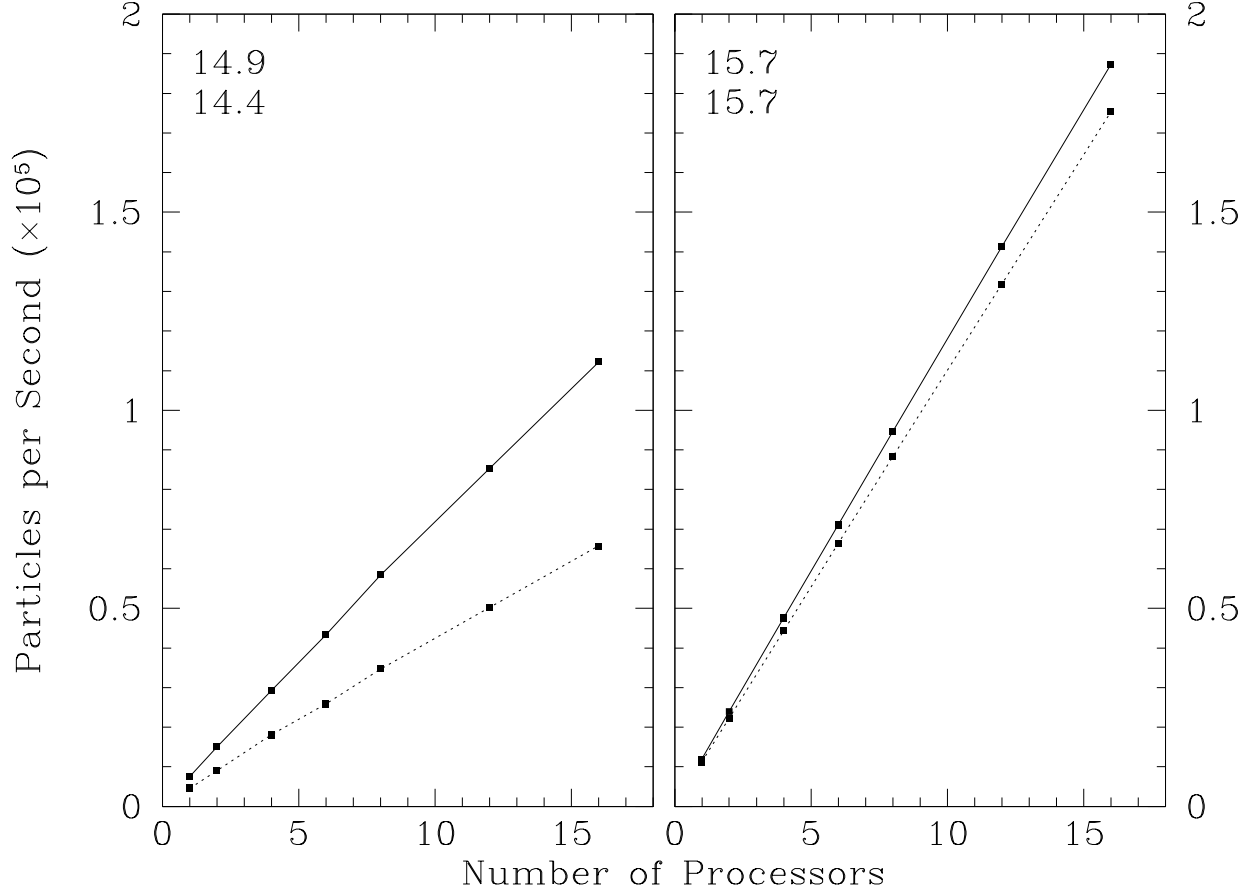


FIG. 18.— Gravitational force calculation rates obtained using VINE on the Power 5 architecture. As in the lowest two panels of figure 8, the left panel shows the performance without the cache blocking algorithm and the right panel shows performance with cache blocking. The solid and dotted curves correspond to runs performed with 16MB pages and with 4kB pages respectively. Scaled parallel efficiency is shown in the upper left corner of each panel for the 16MB (top) and 4kB (bottom) results, out of a machine maximum of 16.

mass, G the gravitational constant and E the total energy. The sphere has a cut-off radius of $r_{max} = 22.8$ and is modeled with $N = 2097152$ particles, using Plummer softening with $\epsilon = 7.6 \times 10^{-3}$. As in FMK05, we use a single GRAPE-6A (‘Micro-Grape’) board, which in our case was attached to an SGI Altix computer with 1.5 GHz Itanium 2 processors.

All tests have been done on a single processor. Reference calculations, against which force accuracy are measured, were performed using either using VINE’s direct summation mode on the host, or alternately with VINE in tree/host mode using a geometric MAC setting of $\theta = 10^{-16}$. Both cases use double precision floating point values, as is standard in VINE. Test calculations using the Gadget MAC use the form defined in equation 9, which provides an estimate of the multipole truncation error at hexadecapole order. An alternate form, described in Springel (2005), implements an opening criterion based on truncation error at quadrupole order, which presumably makes it more appropriate for calculations involving GRAPE. We have chosen not to implement this option however in order to make the tree traversal process as nearly identical as possible between tests with and without GRAPE. In any case, the two

criteria are closely related through the formula

$$\theta_H = \left(\frac{h}{r}\right)^2 \theta_Q, \quad (14)$$

where θ_H and θ_Q are the opening parameter for the hexadecapole and quadrupole based criteria, respectively, r is the separation, and h is the size of the node under consideration. For more liberal settings for which performance is highest, nodes openings will be driven by equation 10, rather than equation 9, so that $h/r \lesssim 1$ and the criteria become identical. For more conservative settings where $h/r < 1$, two parameters become scaled variants of each other. Because we plot calculation rates against force accuracy, rather than against opening parameter, differences in the parameter value with one or the other criterion do not directly affect the comparisons.

7.5.1. Performances as a function of accuracy and problem size

Figure 19 shows the rate of gravity calculations per second as a function of the 50% (i.e. median) and 99% error magnitudes, for the tree/host combination using the Gadget and geometric MACs and the GRAPE-tree combination using only the Gadget MAC. As we saw in figure 3 for parallel calculations on the Origin architecture,

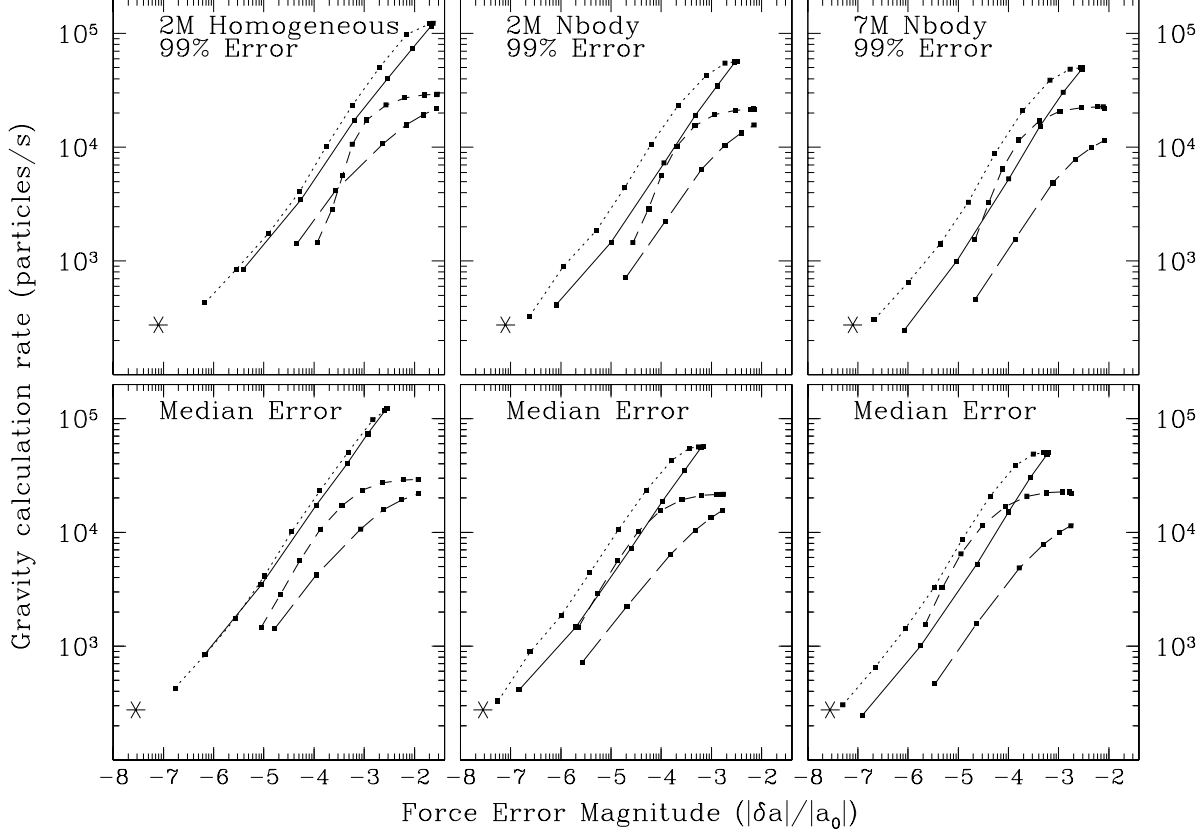


FIG. 19.— The calculation rate for gravitational forces on particles in a homogeneous sphere configuration (left panels) and in the 2 and 7 million particle N -body test problems (center and right panels, respectively). Top panels show rates for which 99% of the particles have error magnitudes less than that shown, while the bottom panels show rates at which 50% (i.e. the median) of particles have errors less than that shown. The solid and dotted curves represent the rates using the geometric MAC and Gadget MACs respectively, both using VINE configured to perform tree+host calculations. The long and short dashed curves represent VINE configured to perform GRAPE-6A+tree calculations using the geometric and Gadget MACs, respectively. Points on each curve represent settings of $\theta = (0.1, 0.2, 0.4, 0.6, 0.8, 1.0)$ for the geometric MAC tests and $10^{-9} \leq \theta \leq 1.0$ in decade increments for the two calculations with the Gadget MAC. The single asterisk in each panel shows the speed and accuracy locus of the GRAPE-6A running in direct summation mode. Labels on the x axis define the exponent of the force accuracy only, rather than the full numerical value, in order to avoid confusion.

using the Gadget MAC allows superior performance relative to the geometric MAC at the same force accuracy, both for the tree/host combination and the GRAPE/tree combination. In no case do error limits rise above 1-2%, even for the most liberal MAC settings, for which several points lie essentially on top of each other in the figure. Only for the homogeneous sphere test, do the error levels rise to this level—for the other two tests, the upper limits are reached at a factor of 2-4 smaller errors. The overall trends for the tree/host calculations closely resemble those seen in figure 3, except for a smaller difference between the behavior of the two MACs in the homogeneous sphere problem here, and the SPH initial condition above, presumably because of the relatively smaller value of the softening length in the present case. Quite different behavior occurs in the GRAPE-6A+tree curves, especially with the Gadget MAC, in which an essentially flat performance plateau exists over nearly an order of magnitude in error limits.

Rates as high as 120kparticles/s are obtained for the homogeneous sphere configuration and >50 kparticles/s for the two N -body test problem configurations.¹¹ In ev-

ery case, the tree/host calculation rates rise to values well above those of the GRAPE-6A+tree rates for the same error limits. Also, the GRAPE-6A+tree curves produce much higher error limits for a given MAC setting than do the tree/host versions, ultimately yielding error limits a factor 2-3 larger at the most liberal MAC settings. The differences are the consequences of two effects which may partially, but incompletely, offset each other. First, while the tree/host calculations includes quadrupole contributions in each interaction, the GRAPE-6A+tree calculations include only the monopole term, so that difference of one order in truncation error in the multipole expansion exists. Larger errors at a given setting are expected as a result. Secondly, many more particle-particle interactions will typically be included in the GRAPE-6A+tree calculations because bunch sizes optimal for this method are much larger than the optimal clump sizes used in the tree/host method. Smaller errors at a given setting are expected in this case, since the particle-particle contributions contribute nothing to the total error. Taken

problem rise lie some 10% higher here than in figure 16 because the present calculations use Plummer softening, in order to compare more directly to the GRAPE calculations, rather than fixed softening length spline softening.

¹¹ Note however that the rates for the 7M particle N -body test

together, clearly the loss of accuracy due to the lower truncation order dominates.

For error limits similar to those produced with the tree/host calculation using the Gadget MAC, for which we use the $\theta = 5 \times 10^{-3}$ setting derived in section 7.2.3 as our reference, the GRAPE-6A+tree calculation requires a setting of $\theta \approx 1 \times 10^{-4}$. Coincidentally, both settings produce the most restrictive accuracy limits for negligible decreases in performance below more liberal settings. For the geometric MAC, equivalent accuracy in the tree/host calculation requires a setting of $\theta \approx 0.75$, while the GRAPE-6A+tree tests require a value $\theta \approx 0.5$. When used in VINE with these settings, the tree/host option in the N -body tests are a factor of about two faster, producing error limits below a few $\times 10^{-3}$ for 99% of the particles, while in the homogeneous sphere test, the tree/host calculations are nearly a factor of four faster.

Though computationally costly, we have extended the high accuracy end of each error curve in figure 19 to relative errors as small as $10^{-8} - 10^{-7}$ for the tree/host settings. Although the settings for which these limits would be obtained would rarely (if ever!) be used in practice, they serve another purpose here. Namely, they allow us to make comparisons between VINE, used in tree/host mode, at the same accuracy as GRAPE-6A processors, used in direct summation mode. Calculations rates for VINE used in tree/host mode with a setting of the Gadget MAC of $\theta \sim 10^{-9}$ typically fall within a factor of $\sim 2 - 3$ of the calculation rates for the GRAPE-6A processor used in direct summation mode.¹² In each case, GRAPE-6A in direct summation mode is the faster option and provides superior absolute performance. It is of interest to note however that the performance advantage is not overwhelmingly large and, when factors such as code complexity and hardware cost are considered, becomes even less so. Assuming host and GRAPE processor are of equal cost, performance when using GRAPE must be at least twice that of the host alone in order to provide a more cost effective solution to a given problem. By this metric, direct summation using GRAPE-6A VINE and host/tree VINE running in parallel on 2-3 host processors, provide roughly equivalent performance.

As a final test of the performance of VINE with GRAPE, we compare the calculation times obtained by using the code in GRAPE-6A direct summation mode, in GRAPE-6A+tree mode and tree+host mode as a function of the size of the problem, again using variants of the N -body test problem. Figure 20 shows the time required to compute gravitational forces with VINE using GRAPE-6A direct summation mode, GRAPE-6A+tree mode and host+tree mode, each as a function of the number of particles in our N -body test problem. Times for the latter two variants are derived using the settings defined above which, as nearly as possible, reproduce the error distributions with similar accuracy constraints. As

¹² Note that because calculations on the GRAPE-6A are done using fixed point arithmetic, with some intermediate operations performed with fewer than the full 64-bits expected on a host processor (Makino et al. 2003), the error limits determined for the GRAPE-6A typically lie near values of a few $\times 10^{-8}$, rather than $\sim 10^{-15}$ expected from double precision floating point limits standard on the host processor. Such direct summation calculations on the host, performed in order to obtain reference values for the force calculations, yield rates of ~ 20 - $30\times$ slower than the GRAPE-6A.

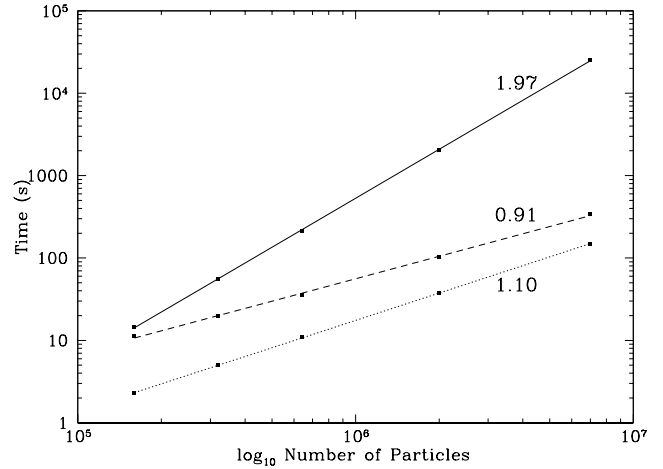


FIG. 20.— Time required to compute gravitational forces of all particles on each other as a function of problem size, for three alternative calculation methods employed in VINE. The three lines correspond to the time required for the GRAPE-6A direct summation option (solid), the GRAPE-6A+tree option (dashed) and the tree/host option (dotted). Each line is a linear fit to the times defined by the points immediately adjacent to it. The slope of each fit is included next to each line.

we expect from basic theoretical considerations of the costs of directly summing the gravitational forces of particles on each other, the slope of the GRAPE-6A direct summation lies very near its predicted value of two. The small deviation below the expected slope is readily explainable if we account for the communication costs of sending and receiving information between the GRAPE-6A and the host. While negligible at large problem sizes, they account for some 5% of the total time for the smallest problem size.

Of greater interest are the two other curves, for GRAPE-6A+tree and for tree/host. While the slope for the tree+host calculation falls quite near the expected $N \log N$ behavior (see also section 7.3.6 and figure 14), the slope for the GRAPE-6A+tree variant lies well below it—below even a linear proportionality. While it seems paradoxical to combine an algorithm whose performance is formally $\mathcal{O}(N_p \log N_p)$ (i.e. tree traversal based force calculations) with another whose performance is formally $\mathcal{O}(N_p^2)$ (i.e. direct summation) and obtain one whose performance is better than $\mathcal{O}(N_p)$, the paradox is readily explainable. Due to the calculation speed of GRAPE hardware, communication costs dominate if the number of calculations is not too large. The turnover towards the expected $\mathcal{O}(N^2)$ scaling takes over only for interaction lists longer than a few 10^4 . As will be shown below in section 7.5.2, VINE's tree traversals reduce the number of interactions per particle to well below this limit and are extremely fast in and of themselves, so we are clearly in a communication dominated performance regime. This conclusion is also confirmed more directly by measurements of the portions of the calculation in which communication occurs. Formally, and as predicted by arguments in Athanassoula et al. (1998); Kawai et al. (2000) and others, the communication dominated regime should scale linearly with problem size, in contradiction to our finding. We note that their arguments neglect the possibility that the optimal bunch population will change as a function of problem size and, though we have made

no specific investigation of the sensitivity of scaling to this parameter, we make the tentative conclusion that this factor is responsible for the effect we see.

At all problem sizes in our study, the performance of the tree/host calculation exceeds that of both the GRAPE-6A direct summation, and the GRAPE-6A+tree option in VINE. Given the clearly different scaling behavior of the two methods however, this statement will not remain true for all problem sizes. The magnitude of the performance difference, even for the largest problem sizes in our study, indicate that the crossover point lies at problem sizes of several tens of millions of particles, a scale at which other factors, such as parallel operation of the code, will play a much larger role in determining the optimal computational method. Superior performance of a tree-based method over that of direct summation is more or less to be expected for all but the smallest problems of course, since the algorithms and the accuracies obtained from them are so different. On the other hand, superior performance of the tree/host calculations over the GRAPE/tree calculations in VINE may not be as readily accepted, since GRAPE hardware is specially designed and optimized to be an efficient gravitational force solver and, as discussed in FMK05, the GRAPE-6A hardware specifically for operation in conjunction with tree based methods. The excellent performance of VINE in tree/host mode demonstrates that careful attention to details of code optimization can overcome such advantages. We caution however, that before concluding that VINE in tree/host mode provides a equal or better alternative to the use of GRAPE hardware, several other factors must be accounted for, each of which will be addressed in the next section.

7.5.2. *Reconciling inconsistencies between the results of our tests and those of Fukushima et al. (2005)*

In section 7.5.1 we found that the performance of VINE's GRAPE-6A+tree combination was substantially slower than that using its tree/host combination at the same accuracy. A closer examination of the timings reveals that the performances is also substantially slower than that quoted in FMK05 as well—while they quote timings of ~ 15 -20 s for force calculations in the homogeneous sphere configuration, our best times were no better than ~ 72 s. Before concluding that force calculations using VINE on a host processor are indeed faster than those using VINE in combination with GRAPE-6A or, more generally, any other code in combination with GRAPE, we must understand the origin of the differences between their timings and our own.

Since communication costs dominate the computation rate, the most obvious possible explanation of the discrepancy is that VINE requires a far larger data volume per interaction to be transferred to the GRAPE than does the code used in FMK05. Here, we show that differences in data transfer volumes are in fact responsible for essentially all of the measurable performance differences. They originate in two important differences between VINE and the FMK05 code: the total number of nodes sent to the GRAPE board for one force calculation, and the volume of data sent per node.

We discuss the latter difference first. The data required for the GRAPE-6A to compute the force due to a given source node minimally include the three components of

its position and its mass. In addition, the GRAPE-6A also requires a node index, to avoid potential self interactions between source and sink nodes, a destination board identifier and a memory address to define where the node will be stored on that board. VINE utilizes the 'g6a' communication library included as the software component of the GRAPE-6A distribution. Communication done using this library also transfers three components of velocity for each node as well as a number of data related to the derivatives of acceleration, which were saved from calculations at previous time steps. In total, 18 words (72 bytes) of data are transferred per node using this library, though the library calls actually used in VINE set the values of many quantities to zero.

In contrast, an alternate library, referred to in the distribution as the 'g65' library, provides an emulation layer for codes written to use calls to a previous generation library distributed with the GRAPE-5 hardware. Most significantly in the present context, this library requires that only the minimal set of data be transferred to the GRAPE-6A for each node, and uses reduced precision for the data that are sent so that the communication cost is reduced to 6 words (24 bytes) per node. In spite of several independent attempts by two of the present authors, we were unable to successfully implement code in VINE to take advantage of the emulation library, although code successfully interfacing directly with the GRAPE-5 library is known to function correctly in VINE. Our tests therefore reflect the higher costs of the full 'g6a' library, with its comparatively inefficient communication. In contrast, tests done in FMK05 implemented code to call the emulation library (2007, T. Fukushima: personal communication), and so reflect a communication cost per node sent which is three times smaller than our own. Differences in communication cost translate to a factor somewhat less than three in speed, because while the costs of tree traversals on the host and computation on the GRAPE-6A are comparatively small, they are not entirely negligible. We will discuss additional implications of this important difference below.

Even accounting for the difference in data volume per node sent, inconsistencies in timings remain between our tests and FMK05. The remaining factors for which we have not accounted are differences in the total number of nodes transferred by each code. Is the total number of nodes sent to the GRAPE in our tests much larger than in the tests performed in Fukushima et al. (2005)? Unfortunately, this question is difficult to answer with precision because the tree construction and traversal algorithms in our code and theirs are quite different. We cannot expect the interaction list lengths obtained for the force calculation on a given bunch to be similar, nor can we expect the average bunch populations to be identical. While one algorithm may produce shorter interaction lists, it may also produce much different force accuracies as a consequence, or may require many more total nodes be sent to the GRAPE because the bunches themselves are not as large. Fukushima et al. (2005) provide timing data only as a function of the (in their case, geometric) MAC setting itself, rather than the accuracy limits provided by that setting. Therefore, comparisons of similar calculations cannot be made. Nevertheless, we will be able to draw some important conclusions from

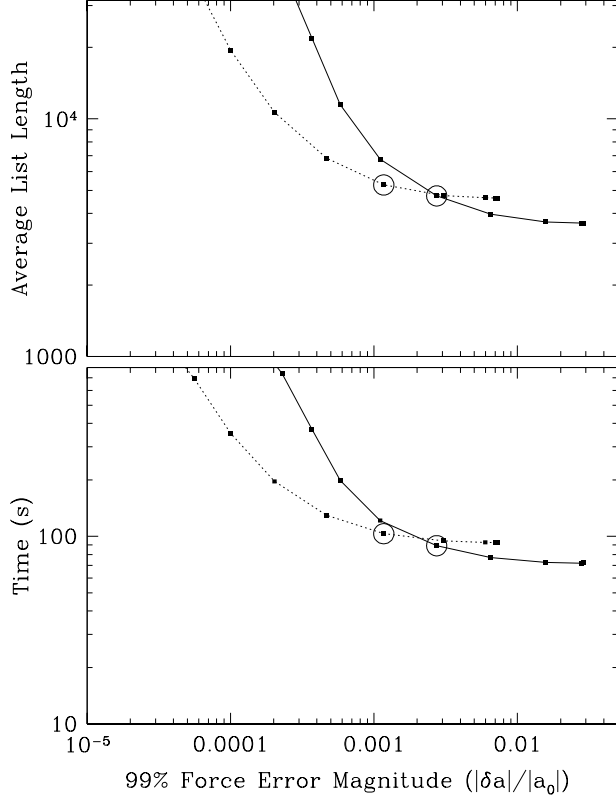


FIG. 21.— Top panel: The average length of the interaction list for each bunch sent to the GRAPE-6A for the homogeneous sphere and the 2M particle N -body test problem, each using the Gadget MAC with the same settings as were used in figure 19. Bottom panel: the time required for a full force calculation on all particles for the same configurations. Solid curves characterize the homogeneous sphere configuration, while dotted curves define the 2M particle N -body test problem configuration. The circled points in each curve denote the location defined by the MAC setting of $\theta = 1 \times 10^{-4}$, recommended above.

the analysis, so we will proceed.

Figure 21 shows the average length of the interaction lists and computation time, each as a function of the 99% limit on force accuracy, using the Gadget MAC. Values for the geometric MAC are larger and are not shown. If we assume that the near flat performance plateau at and above our recommended Gadget MAC setting of $\theta = 1 \times 10^{-4}$ corresponds to a similar feature in figure 5 of FMK05, between $\theta \approx 0.7$ and $\theta = 1$, using a geometric MAC, then we may gain some insight into the performance differences by comparing values derived from our figure and theirs.

For both configurations, the average interaction list lengths at the most liberal MAC settings begin near 3850 and 4650 nodes per bunch for the homogeneous sphere and N -body test problem, respectively. The lengths increase some 10-20%, to near 4750 and 5280 nodes per bunch at our recommended MAC setting and thereafter increase much more rapidly, similar to the behavior seen in FMK05. In comparison to the values of ~ 3200 nodes per bunch quoted for their recommended geometric MAC setting of $\theta = 0.75$, ours are some $\sim 50\%$ larger. Also, in comparison to their average bunch population of 836 (obtained from their Table 2), ours are smaller, near 600 particles per bunch. In combination, the two quanti-

ties determine the total number of nodes sent to the GRAPE-6A, and a simple calculation leads to the result that VINE requires slightly more than twice the number of nodes be sent to the GRAPE-6A than does the code used by FMK05.

7.5.3. Final notes on GRAPE+tree performance in VINE

Naively multiplying together the factor of ~ 2 difference in node count sent to the GRAPE-6A by VINE with the near factor of three difference in data volume per node, we arrive at a potential speed difference of a factor of as large as ~ 5 -6 between the GRAPE-6A+tree code used in VINE compared to that in FMK05. This value is quite consistent with the differences in overall timings at the fastest rates quoted in their work and ours, though ambiguity remains regarding timing comparisons for forces computed to greater or lesser accuracy. This consideration may be of some significance because of our finding in section 7.5 that the geometric MAC setting of $\theta = 0.5$ is required to obtain force accuracies similar to those found for optimal settings in VINE with the Gadget MAC. Calculation rates derived from the FMK05 analyses decrease by a nearly factor of two with this setting as compared to their optimal rates. In the absence of performance tests compared at the same accuracy, we can make no more definitive statements comparing the true relative performance of the two codes.

Nevertheless, we must conclude that as currently implemented in VINE, the GRAPE+tree option is not optimal, due to the inefficient communication arising from our use of the **g6a** library. Users who wish to take full advantage of GRAPE-6A hardware with VINE may be well advised to incorporate appropriate modifications to either the VINE source code or the **g65** emulation library, to enable its successful use. Such modifications have not been a high priority in our work because of the comparatively good performance of the tree/host option. Assuming an ideal factor of three performance enhancement using the reduced communication emulation library, the relative performance compared to VINE in tree/host mode favors the use of GRAPE-6A+tree by only $\sim 50\%$ —a factor much smaller than can be had by simply running the same job on two or more processors in parallel. Such parallelism is highly desirable for the simulations most commonly run in our scientific work, because they are typically much larger than can be completed within the short turn-around time spans required for maximum scientific productivity. They also typically include physical processes (e.g. hydrodynamics with SPH) beyond gravitational effects, which of course cannot utilize the GRAPE hardware but can be efficiently parallelized on the host.

We are hopeful that VINE will be able to demonstrate speedups when using the GRAPE+tree combination in conjunction with future GRAPE hardware currently in development, such as GRAPE-7, as these use faster versions of the PCI bus interface for the data transfer.

8. SUMMARY

In this paper we have described the algorithms used in our particle based numerical code VINE, the optimizations we have made to those algorithms to improve their performance on microprocessor based computers and, finally, a number of benchmarks designed to illustrate the

benefits of each optimization in the most costly calculations required for simulations of astrophysical systems. VINE is written in standard Fortran 95, and is known to compile and run without modification on a variety of common hardware platforms, from small scale desktop workstations to large scale shared memory parallel supercomputers. It realizes excellent performance on both, in both serial and parallel operation. It includes options to model a number of basic physical processes commonly required in models of astrophysical systems, and has been designed to be extensible, so that including additional physical processes in models will be comparatively straightforward.

Although we believe that many members of the computational astrophysics community would benefit from using VINE as an important or primary component of their computational tool box, we recognize that others with substantial investments in other codes might prefer to continue working with them instead. We believe that such users will not find great difficulty in either porting their physical models to VINE and using it as an alternative to verify or otherwise check results from their own codes, or in modifying their codes to include many of the optimizations described here, providing benefits of similar magnitude.

8.1. Overall performance and scaling

We have discussed the performance and scalability of various components of the code in great detail, but have left questions of the scalability of the code as a whole to Vine1. Nevertheless, some comments are relevant here as well. We are very encouraged to see that the parallel scalability of the gravity and SPH calculations are excellent. Also, though we have made no specific study of it, performance appears to remain good even when the code is used in an environment where only a small fraction of particles require forces on any given time step update.

Nevertheless, there are features which limit VINE's performance, of which its users should be aware. Perhaps the most important are the current costs of tree builds and revisions and their parallel scalability. Even though comparatively small in absolute cost, these operations may become expensive when VINE is used in conjunction with individual time steps because their cost is the same, no matter how many particles are updated. They may also become comparatively more costly in massively parallel operation, if VINE were run on hundreds of processors. In studies not detailed here, we have found that when significant populations of particles are present in $\gtrsim 12$ time step bins (i.e. a factor of ~ 4000 difference in δt), tree updates become comparable to force evaluation costs on a moderately parallel (32-64 processor) ~ 3 million particle simulation. Costs and scaling will improve as simulation size increases of course, but cannot entirely be removed.

8.2. Additional Optimization

VINE is very well optimized for high performance and includes many features, but it is a programming truism that no code is ever complete. VINE is no exception, and there are a number of areas where it could be made more flexible, or its performance could be improved. In Vine1, we discussed additional optimizations that may benefit the code at a comparatively high level, such as changes

to the integrators used. Here, we discuss a number of additional, lower level optimizations that we believe may be beneficial to VINE users.

The two most costly components of VINE are the gravity and SPH calculations. For gravity, the optimizations most likely to be beneficial will be from including additional terms in the multipole summation, which is currently truncated at quadrupole order. Including terms to octupole or hexadecapole order would increase the accuracy of the calculation for a given MAC setting, but would also increase the cost of the calculation both in memory and in time. Indirectly, the additional terms will increase the cost to update the nodes in a tree revision, already a comparatively inefficient component of the code. In order to be beneficial, increased accuracy must be both necessary for the calculation and require less total cost to achieve than with the present code used with a more restrictive MAC setting. Because models of many astrophysical systems require force accuracies of only 0.1–1%, for which the speed of the calculation is already at its maximum, the actual benefit will be minimal. To date, we have therefore not implemented such higher order terms. Salmon & Warren (1994) demonstrate that for higher accuracy requirements, including higher order multipole moments will be beneficial and when such accuracy is required, we would recommend their inclusion.

We saw in section 7.3.6 that the parallel performance of the SPH calculations saturated at a factor ~ 50 speedup in the Merger test simulations in which both SPH and N -body particles were present. In part, we attributed the comparative performance loss, relative to the pure SPH test problems, to the fact that both SPH and N -body particles shared the same tree structure, with only a small fraction of the total modeling the gas as SPH particles. In this context, a useful optimization would be to separate each particle species into a distinct tree structure. Then, tree traversals required to obtain neighbor information would require far fewer node examinations, and load balancing between different processors would be less sensitive to the specific distribution of particles in the tree. We estimate that building separate trees for particles of different types would improve the SPH calculation rate by roughly a factor of two in the Merger simulations. We have not implemented such separation because benefits will only be substantial when SPH particles are a small fraction of the total, so that the total computation time is less significant.

Of the four major components of the code described in this paper, the performance of the tree build and revision scale with least efficiency to large processor counts. They can therefore represent a significant proportion of the total time required to complete a given simulation, especially when the option to use individual time steps for each particle is active. Even though the cost of a single call to either component is small, that cost is constant no matter how many particles are updated, so that their cost relative to the average number of particles updated per call can be high. Further optimizations that remedy their performance limitations will therefore be of greatest benefit in speeding up entire simulations.

In the case of the tree revision, essentially all of the cost is contained within a single traversal of the data arrays holding the position, mass and multipole moment information for each node. Similar performance bottlenecks

occur for other simple loops like those that perform particle extrapolations and updates, and are due largely to the variable memory latencies (‘NUMA’—see section 2.3) intrinsic to large scale shared memory architectures. Unfortunately however, we have already mined the area of memory layout optimizations and further improvements from these techniques are not likely to yield additional benefits. Instead, a more profitable optimization will likely be to update only parts of the tree corresponding to active regions of the calculation, rather than its entirety. The benefit will not come without cost however because partial updates mean increased levels of error in the calculations that depend on the tree data, and some very fast technique must be developed to define which parts of the tree are active enough to require a full update, and which may be left for later.

Parallel performance of the tree construction also saturates at factors of $\sim 10 - 12$, but for other reasons than memory latency. In present form, some portions of the build remain un-parallelized, of which the operations involved in assigning particles to specific hash grid zones comprise the largest fraction, at $\sim 1 - 2\%$ of the total build time on one processor and correspondingly more in parallel operation. While nominally parallelizable, attempts to do so resulted in particularly poor scaling and actual slow downs relative to serial performance and have therefore been disabled. Alternative assignment strategies that improved this scaling would yield immediate benefits in the overall scaling of the build.

Secondarily, it may be beneficial to dynamically adjust the hashing factor used to assign particles to the temporary grid according to whether the particle distribution is particularly smooth or particularly inhomogeneous. A low average number per zone will benefit highly inhomogeneous distributions, where a few zones may contain a very large number of particles while many others remain empty. A high average number per zone will benefit smooth distributions where the cost of expanding the search volume increases relative to the cost of examining a single zone. Finally, due to the modular structure of the tree build and tree traversals, it is possible to replace the binary tree currently implemented with another structure to serve the same purpose, so long as a similar post-processing step can be taken to establish identical

relationships between nodes on any right branch of the tree and their parent node’s sibling, as described in section 3.5. Whether any of these changes will be of net benefit is unknown.

8.3. Availability of the code

The code is available to the public under GNU General Public License version 2, via download from the ApJS website, directly from the authors or via download at the USM website: <http://www.usm.lmu.de/people/mwetz> and at both <http://arXiv.org/abs/0802.4245> and <http://arXiv.org/abs/0802.4253>, by choosing the “Other Formats” sub-link and then “Download Source”.

We wish to thank Willy Benz for his generous gift to so many, over so many years, of his SPH wisdom and the original code on which VINE is based. We also wish to thank the referee, Volker Springel, for his comments on this manuscript. Some of the computations reported here were performed using the UK Astrophysical Fluids Facility (UKAFF), on which this code was largely developed, and to whom AFN owes gratitude for financial support. AFN wishes to thank UKAFF system administrators Chris Rudge and Richard West for their helpful and continued cooperation with changes to system configuration that enabled various performance tests to be made during the development of this code. Portions of this work were performed on the SGI-Altix 3700 Bx2 supercomputer at the University Observatory, Munich, which was partly funded and is supported by the DFG cluster of excellence “Origin and Structure of the Universe” (www.universe-cluster.de). Portions of this work were carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396, for which this is publication LA-UR 08-0430. Some of the computations presented here used facilities at the Rechenzentrum Garching of the Max-Planck-Gesellschaft. We wish to thank Matthew Bate for making a set of initial conditions for our SPH tests runs available to us. MW acknowledges financial support by Volkswagen Foundation under grant I/80 040.

REFERENCES

- Anderson, R. J. 1999, *SIAM J. Comput.*, 28, 1923
 Athanassoula, E., Bosma, A., Lambert, J.-C., & Makino, J. 1998, *MNRAS*, 293, 369
 Barnes, J. 1990, *J. Comp. Phys.*, 87, 161
 Barnes, J. E. & Hut, P. 1986, *Nature*, 324, 446
 Bate, M. R., Bonnell, I. A., & Bromm, V. 2003, *MNRAS*, 339, 577
 Bell, E. F., Naab, T., McIntosh, D. H., Somerville, R. S., Caldwell, J. A. R., Barden, M., Wolf, C., Rix, H.-W., Beckwith, S. V., Borch, A., Häussler, B., Heymans, C., Jahnke, K., Jogee, S., Koposov, S., Meisenheimer, K., Peng, C. Y., Sanchez, S. F., & Wisotzki, L. 2006, *ApJ*, 640, 241
 Bentley, J. L. 1979, *IEEE Transactions on Software Engineering*, SE-5, v4, 333
 Benz, W., Bowers, R. L., Cameron, A. G. W., & Press, W. H. 1990, *ApJ*, 348, 647
 Deagum, L. & Menon, R. 1999, *IEEE Computational Science and Engineering*, 5(1), 46
 Dubinski, J. 1996, *New Astronomy*, 1, 133
 Dubinski, J., Kim, J., Park, C., & Humble, R. 2003, *New Astronomy*, 9, 111
 Fukushige, T., Makino, J., & Kawai, A. 2005, *PASJ*, 57, 1009
 Goldberg, D. 1991, *ACM Computing Surveys*, 23, 5
 Herant, M. & Woosley, S. E. 1994, *ApJ*, 425, 814
 Hernquist, L. 1990a, *ApJ*, 356, 359
 —. 1990b, *J. Comp. Phys.*, 87, 137
 —. 1993, *ApJS*, 86, 389
 Hockney, R. W. & Eastwood, J. W. 1981, *Computer Simulations Using Particles* (McGraw-Hill Inc.)
 Ito, T., Ebisuzaki, T., Makino, J., & Sugimoto, D. 1991, *PASJ*, 43, 547
 Jernigan, J. G. & Porter, D. H. 1989, *ApJS*, 71, 871
 Kawai, A., Fukushige, T., Taiji, M., Makino, J., & Sugimoto, D. 2000, *PASJ*, 52, 659
 Makino, J. 1990a, *J. Comp. Phys.*, 88, 393
 —. 1990b, *J. Comp. Phys.*, 87, 148
 —. 1991, *PASJ*, 43, 621
 Makino, J., Fukushige, T., Koga, M., & Namura, K. 2003, *PASJ*, 55, 1163
 Makino, J., Ito, T., & Ebisuzaki, T. 1990, *PASJ*, 42, 717
 Makino, J. & Taiji, M. 1998, *Scientific Simulations with Special-Purpose Computers : The GRAPE Systems* (Chichester, Toronto: John Wiley & Sons)
 Makino, J., Taiji, M., Ebisuzaki, T., & Sugimoto, D. 1997, *ApJ*, 480, 432

- Naab, T. & Burkert, A. 2003, *ApJ*, 597, 893
- Naab, T., Jesseit, R., & Burkert, A. 2006a, *MNRAS*, 372, 839
- Naab, T., Khochfar, S., & Burkert, A. 2006b, *ApJ*, 636, L81
- Okumura, S. K., Makino, J., Ebisuzaki, T., Fukushige, T., Ito, T., Sugimoto, D., Hashimoto, E., Tomida, K., & Miyakawa, N. 1993, *PASJ*, 45, 329
- Press, W. 1986, in *Lecture Notes in Physics*, Vol. 267, *The Use of Supercomputers in Stellar Dynamics*, ed. P. Hut & S. McMillan, Institute for Advanced Study, Princeton, USA (Springer-Verlag, Berlin Heidelberg New York), 184–192
- Salmon, J. K. & Warren, M. S. 1994, *J. Comp. Phys.*, 111, 136
- Sanders, P. & Hansch, T. 1997, in *IRREGULAR '97: Proceedings of the 4th International Symposium on Solving Irregularly Structured Problems in Parallel* (London, UK: Springer-Verlag), 13–24
- Springel, V. 2005, *MNRAS*, 364, 1105
- Springel, V., Yoshida, N., & White, S. D. M. 2001, *New Astronomy*, 6, 79
- Stadel, J. 2001, PhD thesis, University of Washington
- Sugimoto, D., Chikada, Y., Makino, J., Ito, T., Ebisuzaki, T., & Umemura, M. 1990, *Nature*, 345, 33
- Wadsley, J. W., Stadel, J., & Quinn, T. 2004, *New Astronomy*, 9, 137
- Waltz, J., Page, G. L., Milder, S. D., Wallin, J., & Antunes, A. 2002, *J. Comp. Phys.*, 178, 1
- Warren, M. S. & Salmon, J. K. 1995, *Computer Physics Communications*, 87, 266
- Wetzstein, M., Naab, T., & Burkert, A. 2007, *MNRAS*, 375, 805
- Wetzstein, M., Nelson, A. F., & Naab, T. 2008, *ApJS*, 0, 0